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CRYSTAL STRUCTURE OF RIBOSOMAL PROTEIN L11/GTPASE ACTIVATING REGION rRNA AND USES THEREOF

TECHNICAL FIELD OF THE INVENTION

The present invention relates to methods of screening for compounds that inhibit or activate bacterial growth by binding to the complex formed between ribosomal protein L11 and the 23S ribosomal RNA region that interacts with it in vivo.

BACKGROUND

The elongation cycle of protein synthesis is driven by two elongation factors that bind to nearly identical sites on the large (50S) ribosomal subunit (Spahn and Nierhaus, 1998; Wilson and Noller, 1998). EF-Tu delivers aminoacyl tRNAs to the ribosome, whereas EF-G catalyzes the translocation of the ribosome by one codon relative to the mRNA and the concomitant movement of the A and P site tRNAs. Both elongation factors are G proteins, and their interactions with the ribosome are coupled to the binding and hydrolysis of GTP. Like most G proteins, EF-Tu and EF-G are molecular switches that have limited inherent GTPase activity, and they rely on an accessory factor to stimulate activity at the appropriate time. This accessory factor is an integral part of the 50S ribosomal subunit and has usually been referred to as the "GTPase center," but by analogy with the functionally equivalent GAP proteins that stimulate GTPase activity in G-proteins, it seems more appropriate to refer to it as the "GTPase activating region" (hereafter abbreviated as the GAR). Early work on the identification of the molecular components of the GAR implicated a complex between ribosomal protein L11 and a highly conserved 58-nucleotide stretch of 23S ribosomal RNA

(rRNA), nucleotides 1051-1108 in *Escherichia coli* (Schmidt et al., 1981; Thompson et al., 1979). The L11-RNA complex is the target for a family of thiazole antibiotics that includes thiostrepton and micrococcin. Thiostrepton binds essentially irreversibly to 50S subunits (Sopori and Lengyel, 1972) and inhibits hydrolysis of GTP by EF-G (Pestka, 1970; Rodnina et al., 1997), while micrococcin binds to the same complex and stimulates GTP hydrolysis by EF-G (Cundliffe and Thompson, 1981).

Other components of the ribosome have also been implicated in stimulation of GTP hydrolysis by elongation factors. Classical work suggested that protein L7/L12, which together with L10 forms the "stalk" of the 50S subunit that lies adjacent to L11, is involved in stimulation of GTPase activity in EF-Tu (Donner et al., 1978). However, recently it has been shown that protein L7/L12, although essential for stalk formation, is not required for viability in yeast (Briones et al., 1998). The sarcin/ricin loop, a small, highly conserved stem-loop in the 23S rRNA that is known to be essential for ribosome function, has been footprinted by the elongation factors (Moazed et al., 1988), and is also considered a candidate for being part of the GAR. Therefore, it is not yet clear whether the L11-RNA complex *per se* should be considered the GAR, or whether the GAR should be defined as a more extensive region of the 50S subunit. In any event, it appears that the L11-RNA complex is at the heart of the GAR; the complex of L11 with its cognate RNA will be referred to herein as the GAR.

The GAR is one of the most thoroughly characterized RNA-protein complexes. The secondary structure of the RNA was first inferred from biochemical and genetic studies (Glotz et al., 1981; Noller et al., 1981). It consists of a junction of four double-helical stems (Figure 1A). Approximately one-third of the residues in the GAR RNA are very highly conserved. The structure, thermodynamic stability, and ion-binding affinities of the RNA

component have been extensively probed by a variety of biophysical and biochemical techniques; these data suggest that the 1067 and 1095 stem-loops are folded into a compact tertiary structure (Conn et al., 1998; Rosendahl and Douthwaite, 1994). Protein L11 consists of two domains: the C-terminal domain binds tightly to the RNA tertiary structure, while the N-terminal domain is required for the cooperative interaction with thiostrepton (Xing and Draper, 1996). The structure of the C-terminal domain has been determined by NMR techniques (Hinck et al., 1997; Markus et al., 1997). Footprinting studies (Rosendahl and Douthwaite, 1993) have identified regions of RNA involved in the interaction with L11, while NMR chemical shift measurements (Hinck et al., 1997) have identified an RNA-binding surface on the C-terminal domain of the protein.

It is an object of the invention to provide a detailed view of a functionally important protein-RNA complex in the ribosome.

It is also an object of the invention to provide a high-resolution structure of a ribosomal protein-RNA complex.

Yet another object of the invention is to provide new principles of RNA folding, of RNA-protein recognition, and of indirect RNA tertiary structure stabilization.

Yet another object of the invention is to solve the three dimensional structure of L11 complexed with GAR RNA and to determine its structure coordinates.

SUMMARY OF THE INVENTION

The present invention is broadly directed to methods of screening ribosomal protein L11/GTPase activating region (GAR) RNA-modulating compounds by using information from the high-resolution structure of the L11/GAR complex.

The invention encompasses use of the structure coordinates of an L11/GAR crystal to define the atomic details of regions of the L11/GAR complex, such as the GTPase activating region and one or more binding sites of accessory factors, which are target sites for inhibitors or activators.

The invention also encompasses use of the structure coordinates and atomic details of the L11/GAR RNA complex or its co-complexes to design, evaluate computationally, synthesize and use inhibitors or activators of the L11/GAR.

Structure coordinates for L11/GAR RNA complex according to Table II may be modified from this original set by mathematical manipulation. Such manipulations include, but are not limited to , crystallographic permutations, fractionalizations, or inversion of the raw structure coordinates, integer additions or subtractions to sets of the raw structure coordinates, and any combination of the above.

The crystal structure of the GAR allows the screening and design of novel classes of GAR inhibitory or activating compounds with great medical potential, for example, to prevent or stimulate growth of certain bacteria.

The invention encompasses a method for identifying a potential modulator of ribosomal protein L11/GAR activity, comprising the steps of: a) using a three-dimensional structure of the L11/GAR complex as defined by atomic coordinates of the L11/GAR according to FIG. 7; b) employing the three-dimensional structure to design or select the potential modulator; c) providing the potential modulator; and d) contacting the potential modulator with L11/GAR in the presence of an activity to determine the ability of the potential modulator to modulate the activity, for example, L11/GAR activity.

In one embodiment of the invention, the potential modulator is designed de novo.

In another embodiment of the invention, the potential modulator is designed from a

known modulator.

In another emdodiment of the invention, the step of employing the three-dimensional structure to design or select the compound comprises the steps of: a) identifying chemical entities or fragments capable of associating with the L11/GAR; and b) assembling the identified chemical entities or fragments into a single molecule to provide the structure of the potential modulator. Relative to this embodiment, the potential modulator may be designed de novo or designed from a known modulator.

The invention further encompasses a method for screening L11/GAR-binding compounds comprising the steps of: 1) incubating in vitro one or more compounds, a known L11/GAR binding activity and labeled RNA comprising GAR RNA; 2) separating that fraction of the labeled RNA bound to the known L11/GAR binding activity from that fraction of the labeled RNA not bound to the known L11/GAR binding activity; and 3) detecting labeled RNA, wherein a decrease in the level of the labeled RNA bound to the known L11/GAR binding activity in the presence of one or more compounds indicates the binding of one or more of the compounds to L11/GAR.

The invention further encompasses a method for screening L11/GAR-binding compounds comprising the steps of: 1) incubating in vitro one or more compounds, a labeled known L11/GAR binding activity and an RNA comprising GAR RNA; 2) separating that fraction of the labeled known L11/GAR binding activity bound to the RNA from that fraction of the labeled known L11/GAR binding activity not bound to the RNA; and 3) detecting labeled known L11/GAR binding activity wherein a decrease in the level of the labeled known L11/GAR binding activity bound to the RNA in the presence of one or more compounds indicates that one or more of the compounds binds L11/GAR.

In one embodiment of the the method of screening L11/GAR-binding compounds, the

known L11/GAR binding activity is an antibiotic. In another embodiment the antibiotic is micrococcin. In a preferred embodiment the antibiotic is thiostrepton.

In another embodiment of the method of screening L11/GAR-binding compounds, the RNA comprising GAR RNA is contained within a ribosome.

In another embodiment of the method of screening L11/GAR-binding compounds, a plurality of compounds is screened for L11/GAR binding in a plurality of separate, simultaneous assays.

The invention further encompasses a method for screening L11/GAR-binding compounds comprising the steps of: 1) incubating in vitro one or more compounds with a translationally competent cell extract and a translatable RNA; and 2) detecting translation, wherein a decrease in the level of translation indicates binding of one or more of the compounds to L11/GAR.

In one embodiment, the translatable RNA encodes an enzyme and the step of detecting translation comprises detecting the activity of the enzyme.

In a preferred embodiment, the enzyme is luciferase.

In another embodiment, the translatable RNA is poly-U, and the step of detecting translation detects the incorporation of labeled phenylalanine into polyphenylalanine.

In another embodiment, the translationally competent cell extract comprises isolated ribosomes.

The invention further encompasses a method for screening L11/GAR-binding compounds comprising the steps of: 1) incubating in vitro one or more compounds, isolated 70S ribosomes, isolated EF-G and gamma-labeled GTP; and 2) detecting GTP hydrolysis wherein a decrease in GTP hydrolysis indicates one or more of the compounds binds L11/GAR.

The invention further encompasses a method for screening anti-bacterial compounds comprising the steps of: 1) incubating in vitro one or more compounds, a known L11/GAR binding activity and labeled RNA comprising GAR RNA; 2) separating that fraction of the labeled RNA bound to the known L11/GAR binding activity from that fraction of the labeled RNA not bound to the known L11/GAR binding activity; and 3) detecting labeled RNA, wherein a decrease in the level of the labeled RNA bound to the known L11/GAR binding activity in the presence of one or more compounds indicates that one or more of the compounds has anti-bacterial properties.

The invention further encompasses a method for screening anti-bacterial compounds comprising the steps of: 1) incubating in vitro one or more compounds, a labeled known L11/GAR binding activity and an RNA comprising GAR RNA; 2) separating that fraction of the labeled known L11/GAR binding activity bound to the RNA from that fraction of the labeled known L11/GAR binding activity not bound to the RNA; and 3) detecting labeled known L11/GAR binding activity wherein a decrease in the level of the labeled known L11/GAR binding activity bound to the RNA in the presence of one or more compounds indicates that one or more of the compounds has anti-bacterial properties.

In one embodiment of the the method of screening anti-bacterial compounds, the known L11/GAR binding activity is an antibiotic. In another embodiment the antibiotic is micrococcin. In a preferred embodiment the antibiotic is thiostrepton.

In another embodiment of the method of screening anti-bacterial compounds, the RNA comprising GAR RNA is contained within a ribosome.

In another embodiment of the method of screening anti-bacterial compounds, a plurality of compounds is screened for L11/GAR binding in a plurality of separate, simultaneous assays.

The invention further encompasses a method for screening anti-bacterial compounds comprising the steps of: 1) incubating in vitro one or more compounds with a translationally competent cell extract and a translatable RNA; and 2) detecting translation, wherein a decrease in the level of translation indicates that one or more of the compounds has anti-bacterial properties.

In one embodiment, the translatable RNA encodes an enzyme and the step of detecting translation comprises detecting the activity of the enzyme.

In a preferred embodiment, the enzyme is luciferase.

In another embodiment, the translatable RNA is poly-U, and the step of detecting translation detects the incorporation of labeled phenylalanine into polyphenylalanine.

In another embodiment, the translationally competent cell extract comprises isolated ribosomes.

The invention further encompasses a method for screening anti-bacterial compounds comprising the steps of: 1) incubating in vitro one or more compounds, isolated 70S ribosomes, isolated EF-G and gamma-labeled GTP; and 2) detecting GTP hydrolysis wherein a decrease in GTP hydrolysis indicates that one or more of the compounds has anti-bacterial properties. Further features and advantages of the invention are embodied in the following description of the invention and in the claims.

BRIEF DESCRIPTION OF THE DRAWINGS

Figure 1 shows an overview of the secondary and tertiary structure of the GTPase activating region RNA from *Thermotoga maritima*: a) RNA secondary structure derived from the crystal structure. Lines indicate long-range base triples and the long-range 1088-1060 base pair; b) ribbon-and-stick schematic of the RNA tertiary structure (For clarity, protein L11 has

been omitted from view); c) same as (b), but the view is down the major groove of the 1095 stem to emphasize the compactness of the RNA fold. Figures 1b and 1c were made with the program RIBBONS (Carson, 1991).

Figure 2 shows selected details of the tertiary structure of the GTPase activating region RNA from *Thermotoga maritima*; in (a) and (b), the RNA backbone is represented by a ribbon and the phosphates are not shown: a) the ribose zipper that mediates the minor-groove to minor-groove association of the terminal stem and the 1082 hairpin loop (Hydrogen bonds are indicated by dotted lines); b) the major-groove to major-groove association of the 1067 and 1095 stem-loops, in a view emphasizing the high-five, S-turn, and dinucleotide platform motifs. The high-five motif consists of the long-range stacking of two bulged residues, U1061 and A1070. The S-turn comprises the inverted nucleotide U1060 and the bulged residue U1061. The dinucleotide platform motif consists of G1089 and U1090, on which the bulged residues G1071 and C1072 rest, as part of the long-range triples G1071-(G1091-C1100) and C1072-(C1092-G1099).

c) Geometries of the noncanonical base pairs and base triples. Top panel, the three major groove base triples in the core of the structure: G1089-(U1090-U1101), G1071-(G1091-C1100), and C1072-(C1092-G1099). Bottom left panel, the minor groove docking interactions (U1082-A1086)-(G1056-A1103) and A1085-(G1054-C1104). Bottom right panel, the long-range pair A1088-U1060. Figures 2a and 2b were made with RIBBONS (Carson, 1991); 2c with MOLSCRIPT (Kraulis, 1991).

Figure 3. RNA-metal ion interactions in the tertiary structure of the GTPase activating region

RNA from *Thermotoga maritima*: a) overview of the locations of the metal ions, showing that they are primarily in the interacting major grooves of the 1067 and 1095 stems. Magnesium ions are gold, cadmium ions are magenta, and the mercury ion is rose. b) close-up of the central cadmium ion that stabilizes sharp turns at the 1056-1057 and 1086-1087 phosphodiester linkages at the center of the 4-way junction. Direct ligation of the cadmium ion is indicated by solid lines, and second-shell ligation is indicated by dotted lines. Figure 3a was made with RIBBONS (Carson, 1991), and Figure 3b was made with MOLSCRIPT (Kraulis, 1991).

Figure 4 shows the RNA-L11 complex within the GTPase activating region from *Thermotoga maritima*: a) alignment of four widely divergent L11 sequences, together with a schematic of the protein's secondary structure. The sidechains of residues colored green participate in the hydrophobic core in the crystal structure. Residues involved in RNA binding are colored blue for side-chain contacts, red for main-chain contacts, or purple if both the side-chain and main-chain interact with RNA. Abbreviations: E. coli, *Escherichia coli* (eubacterium); T. marit, *Thermotoga maritima* (eubacterium); Sulf ac, *Sulfolobus acidocaldarius* (archaea) ; Sacc cer, *Saccharomyces cerevisiae* (eukaryote). The numbering is based on the *Thermotoga maritima* sequence present in the crystal structure. b) stereoview of the complex. The L11 N- and C-terminal domains are labeled. Note that the N-terminal domain straddles the interface of the 1067 and 1095 stem-loops. c) orthogonal stereoview of the complex. This view emphasizes the relatively loose association of the L11 N-terminal domain with the RNA. Figures 4b and 4c were made with RIBBONS (Carson, 1991).

Figure 5 shows Protein-RNA recognition within the GTPase activating region from *Thermotoga maritima*: a) schematic of RNA-CTD interactions observed in the crystal structure. Unusual RNA conformational features are also indicated (see inset for key). Water molecules that mediate protein-RNA interactions are indicated by a "W". b) Detail of the recognition of the conserved long-range A1088-U1060 pair by conserved L11 residues Gly130 and Thr131 from helix 5, and by the N-terminus of helix 3. Figure 5b was made with MOLSCRIPT (Kraulis, 1991).

Figure 6 shows that the sites of mutations conferring resistance to thiostrepton and micrococcin are clustered around a cleft between the RNA and the proline-rich helix in the L11 N-terminal domain. Residues implicated in thiostrepton binding (A1067, A1095, and Pro22) are labeled. The position of Tyr61, which is protected by thiostrepton in protein footprinting experiments, is also indicated. Other labeled residues are those that confer micrococcin resistance (see text for details). The figure was made with RIBBONS (Carson, 1991).

Table II shows the atomic structure coordinates for the complex between ribosomal L11 protein and the GAR RNA as derived by X-ray diffraction from a crystal of L11 complexed with 23S rRNA nucleotides 1051-1108.

DETAILED DESCRIPTION OF THE INVENTION

The invention is based on the discovery of the crystal structure of the ribosomal GAR from the hyperthermophilic eubacterium *Thermotoga maritima*, which is disclosed herein.

Definitions:

As used herein, the term "binding site" or "binding pocket" refers to a region of a protein or protein/RNA complex which binds or interacts with a particular compound. It is understood that the composition of the protein or RNA residues and/or the protein or RNA backbone, as well as the interaction of such moieties with their solvent including ions defines the specificity of the binding pocket.

As used herein, the term "exposed residue" refers to an amino acid or RNA residue which is located on the surface of a protein, RNA or RNA/protein complex.

As used herein the term "N terminus" or "N terminal lobe" or "NTD" when used in reference to L11 means amino acids 1-70 of L11.

As used herein, the term "C terminus" or "C terminal lobe" or "CTD" when used in reference to L11 means amino acids 76-141 of L11.

As used herein, the term "tether" or "tether sequence" when used in reference to L11 means animo acids 71 to 75 of L11.

As used herein, the term "flexible" when applied to a protein or RNA domain means that that domain allows one or more domains adjoining or flanking it to move or flex in space relative to the flexible domain.

As used herein, the term "backbone" or "backbone residue" when applied to an RNA molecule refers to the sugar-phosphate moieties that are covalently linked to form an RNA polymer. When applied to a protein molecule, "backbone" or "backbone residue" refers to the alternating N-C-C-N moieties of amino acids that are covalently linked to form a peptide polymer.

As used herein, the term "interface" means the point or surface at which two or more domains of one or more molecules associate with each other.

As used herein, the term "GAR" refers to the region of the ribosome responsible for activating the GTPase activity of translation elongation factors. The term "GAR RNA" refers to nucleotides 1051 to 1108 of E. coli 23S rRNA or to its functional and structurally equivalent from any other bacterial rRNA. As used herein, GAR RNA refers to the nucleotides including and limited to (i.e., an RNA molecule consisting of GAR RNA) nucleotides 1051 to 1108 of E. Coli 23S rRNA (or the functionally and structurally equivalent region in other bacterial rRNAs); or it refers to that nucleotide region (1051 to 1108) within a longer nucleotide sequence (i.e., an RNA molecule consisting essentially of GAR RNA) where the GAR RNA (nucleotides 1051 to 1108) is the only active region in the longer sequence (in terms of binding and/or another activity), whether the extra sequence be a homologous sequence from the 23S rRNA (short of the complete sequence) or a heterologous sequence; or it refers to the 1051 to 1108 region within a complete functional 23S rRNA (i.e., an RNA molecule comprising the GAR RNA).

As used herein, the term "L11/GAR" refers to the portions of L11 and GAR RNA which, when engaged in a complex, provide the L11/GAR binding site and/or activity, and preferably both the binding site and the activity. The term "L11/GAR" refers to a complex which consists of the ribosomal protein L11 and consists of the GAR RNA (nucleotides 1051 to 1108) in their native association; or it can refer to a complex consisting essentially of ribosomal protein L11 and consisting of or consisting essentially of or comprising GAR RNA (i.e., including other proteins which are inactive or do not otherwise affect the activity of the L11/GAR complex; or it can refer to a complex comprising ribosomal protein L11 and consisting of, consisting essentially of, or comprising GAR RNA. When ribosomal protein L11 is referred to, the complete protein is referred to; however, where an L11/GAR activity is referred to, the portion of L11 sufficient to provide the activity when associated in a complex

with GAR ma be less than the complete L11 protein; "portion" referring to those combined L11 residues which provide for L11/GARcomplex formation and activity, the portions being one or more of the N-terminal, C-terminal or tether regions, as defined herein, or ant combination thereof .

"L11/GAR activity" may include one or more of the following: movement of the N-terminal lobe of L11; binding or displacement of thiostrepton or micrococcin; RNA translation, translation elongation, inhibition of amino acid addition, GTPase activity, and/or inhibition of elongation factor G (EF-G)-dependent GTP hydrolysis.

As used herein, the term "known L11/GAR binding activity" refers to an activity known in the art to associate with the L11/GAR either in vitro or in vivo. Known L11/GAR binding activities include, but are not limited to, the binding of agents such as thiostrepton and micrococcin.

As used herein, "stem loop" refers to a stretch of nucleic acid sequence on a single molecule comprising two lengths of sequence capable of forming hydrogen bonded base pairs with each other separated by a region which cannot participate in the same base pairing interaction, such that base pairing between the sequences capable of forming hydrogen bonded base pairs forms a loop of non-base paired nucleic acid consisting of the region which cannot participate in base pairing.

As used herein, the term "alpha helix" refers to a secondary structure arrangement of amino acids wherein hydrogen bonding between the C=O group of one peptide and the -NH group of the peptide bond four residues further down the same peptide polymer results in a right handed twist or helix formation.

As used herein, "four way junction" refers to a region in the tertiary structure of GAR RNA in which four helices interact simultaneously with each other, as defined by the crystal

structure coordinates given in Table II.

As used herein, the term "translationally competent cell extract" refers to any fraction of a cell lysate, including a whole cell lysate, which is capable of directing the RNA-dependent polymerization of peptide bonds.

As used herein, the term "translatable RNA" refers to an RNA which, when incubated with factors necessary for translation can direct the synthesis of acid-precipitable protein.

As used herein, the term "decrease" when used in reference to a level of labeled RNA, a level of known L11/GAR binding activity, a level of translation, or a level of GTP hydrolysis means that the detected level is reduced by at least 10%, and preferably by 20% to 50% or more.

As used herein, the term "anti-bacterial properties" refers to the ability of a particular compound to inhibit the growth of bacteria. A compound can be said to have anti-bacterial properties if the rate of bacterial cell proliferation is reduced by at least 50%, and preferably by more than 50%.

As used herein, the term "naturally occurring amino acids" means the L-isomers of the naturally occurring amino acids. The naturally occurring amino acids are glycine (G, Gly), alanine (A, Ala), valine (V, Val), leucine (L, Leu), isoleucine (I, Ile), serine (S, Ser), methionine (M, Met), threonine (T, Thr), phenylalanine (F, Phe), tyrosine (Y, Tyr), tryptophan (W, Trp), cysteine (C, Cys), proline (P, Pro), histidine (H, His), aspartic acid (D, Asp), asparagine (N, Asn), glutamic acid (E, Glu), glutamine (Q, Gln), gamma-carboxyglutamic acid, arginine (R, Arg), ornithine and lysine (K, Lys). Unless specifically indicated, all amino acids referred to in this application are in the L-form.

As used herein, the term "unnatural amino acids" means amino acids that are not naturally found in proteins. Examples of unnatural amino acids used herein include racemic

mixtures of selenocysteine and selenomethionine.

The term "positively charged amino acid" includes any naturally occurring or unnatural amino acid having a positively charged side chain under normal physiological conditions. Examples of positively charged naturally occurring amino acids are arginine, lysine and histidine.

The term "negatively charged amino acid" includes any naturally occurring or unnatural amino acid having a negatively charged side chain under normal physiological conditions. Examples of negatively charged naturally occurring amino acids are aspartic acid and glutamic acid.

The term "hydrophobic amino acid" means any amino acid having an uncharged, nonpolar side chain that is relatively insoluble in water. Examples of naturally occurring hydrophobic amino acids are alanine, leucine, isoleucine, valine, proline, phenylalanine, tryptophan and methionine.

The term "hydrophilic amino acid" means any amino acid having an uncharged, polar side chain that is relatively soluble in water. Examples of naturally occurring hydrophilic amino acids are serine, threonine, tyrosine, asparagine, glutamine, and cysteine.

As used herein, a "competitive" inhibitor is one that inhibits GAR activity by binding to the same kinetic form of the GAR as its accessory factors bind--thus directly competing with the accessory factors for the active site of the GAR. Competitive inhibition can be reversed completely by increasing the accessory factor concentration.

As used herein, the term “kinetic form” of the GAR means the condition of the GAR when either bound to an accessory factor or not, and in either its active or inactive state. That is, a kinetic form can be any conformation the GAR can assume under physiological conditions.

As used herein, the term "accessory factor" means an endogenous factor or protein that interacts with the L11/GAR. As used herein, EF-G is included in the term "accessory factor".

As used herein, an "uncompetitive" inhibitor is one that inhibits GAR activity by binding to a different kinetic form of the GAR than do the accessory factors. Such inhibitors bind to GAR already bound with the accessory factor and not to the accessory factor-free GAR. Uncompetitive inhibition cannot be reversed completely by increasing the accessory factor concentration.

As used herein, the term "co-complex" means L11 protein in covalent or non-covalent association with GAR RNA. As used herein, a co-complex may also encompass accessory factors and/or inhibitors or activators complexed with L11 or L11/GAR RNA.

As used herein, the terms "associates with" or "interacts with" refers to a condition of proximity between a chemical entity or compound, or portions thereof, with another chemical entity, compound or portion thereof. The association or interaction may be non-covalent --wherein the juxtaposition is energetically favored by hydrogen bonding or van der Waals or electrostatic interactions-- or it may be covalent.

The term "beta-sheet" refers to the conformation of a polypeptide chain stretched into an extended zig-zig conformation. Portions of polypeptide chains that run "parallel" all run in the same direction. Polypeptide chains that are "antiparallel" run in the opposite direction from the parallel chains.

As used herein, the term "target" means a region of the L11/GAR complex, as defined by the crystal structure coordinates of Table II, which when bound by a candidate inhibitor or activator results in inhibition or activation of L11/GAR function.

As used herein, the term "modulate" refers to a change, either an increase or a

decrease in some activity.

As used herein, the term "modulator" means a compound that modulates some activity.

As used herein, the term "inhibits" or "decreases" means that a candidate modulator reduces the activity of the L11/GAR. A candidate modulator may be said to inhibit or decrease activity if the activity of L11/GAR as measured by inhibition of GTP hydrolysis and/or

translational activity is reduced by more than 50% in the presence of 50 uM or less of inhbitor compared to values obtained in the absence of inhibitor. Candidate modulators will preferably inhibit by more than 50% the presence of 10 uM or less of inhbitor and most preferably in

the presence of 1 uM or less of inhibitor.

As used herein, the term "activates" or "increases" means that a candidate modulator raises the activity of the L11/GAR. A candidate modulator may be said to activate or increase activity if the activity of L11/GAR as measured by an increase of GTP hydrolysis by more than 50% in the presence of 50 uM or less of activator compared to values obtained in the absence of activator. Candidate modulators will preferably activate by more than 50% in the presence of 10 uM or less of inhibitor and most preferably in the presence of 1 uM or less of

inhibitor.

As used herein, the term "structure coordinates" refers to mathematical coordinates derived from mathematical equations related to the patterns obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of an L11/GAR RNA complex in crystal form. The diffraction data are used to calculate an electron density map of

the repeating unit of the crystal. The electron density maps are used to establish the positions of the individual atoms within the unit cell of the crystal.

As uded herein, the term "heavy atom derivatization" refers to the method of producing a chemically modified form of a crystal of L11/GAR RNA. In practice, a crystal is soaked in a solution containing heavy metal atom salts, or organometallic compounds, e.g., methyl mercury nitrate, lead chloride, gold thiomalate, thimerosal or uranyl acetate, which can diffuse through the crystal and bind to the surface of the protein. The location(s) of the bound heavy metal atom(s) can be determined by X-ray diffraction analysis of the soaked crystal. This information, in turn, is used to generate the phase information used to construct three-dimensional structure of the protein or protein:RNA complex (Blundel, T. L. and N. L. Johnson, 1976, Protein Crystallography, Academic Press).

Those of skill in the art understand that a set of structure co-ordinates determined by X-ray crystallography is not without standard error. For the purpose of this invention, any set of structure coordinates for an L11/GAR RNA complex that has a root mean square deviation of protein backbone atoms (N, Cα, C and O) of less than 0.75 when superimposed on the structure coordinates of Table II, using backbone atoms, shall be considered identical.

The term "unit cell" refers to a basic parallelipiped shaped block. The entire volume of a crystal may be constructed by regular assembly of such blocks. Each unit cell comprises a complete representation of the unit of pattern, the repetition of which builds up the crystal. Using the structure coordinates of the L11/GAR RNA complex provided by this invention, molecular replacement may be used to determine the structure coordinates of a crystalline mutant or homologue of the L11/GAR RNA complex or of a different crystal form of the L11/GAR RNA complex.

Detailed Description of the High Resolution Structure of the L11/GAR complex.

The GAR RNA from the *T. maritima* 23S rRNA consists of nucleotides 1111-1168, which correspond to nucleotides 1051-1108 in the *E. coli* sequence. Hereafter, the *E. coli* numbering will be used in order to facilitate comparison with the available biochemical and genetic data. As described in detail in Example 1, crystals of the GAR RNA complexed with ribosomal protein L11 from *T. maritima* were prepared and used to solve the structure to 2.6 Å resolution using multi-wavelength anomalous diffraction on a mercury derivative of the crystal. Data collection, phasing and refinement statistics are shown in Table I. The asymmetric unit in the crystal consists of two 1:1 L11-RNA complexes stacked in a head-to-head manner. The two complexes are nearly identical except for a subtle bend in the terminal three base pairs of the RNA, and a difference in the degree of disorder of the two L11 N-terminal domains. Several observations strongly suggest that the conformation observed in the crystal structure is extremely similar to the structure of the GAR *in situ* in the ribosome. The RNA contains all of the predicted secondary structure; the two complexes in the asymmetric unit are virtually identical; and, most significantly, the structure explains most of the large body of experimental data on this system.

Structure of the GAR RNA

The predicted secondary structure of the GAR RNA (Glotz et al., 1981; Noller et al., 1981) is almost identical to that derived from the crystal structure (Figure 1a). The RNA secondary structure contains four double-helical segments, referred to as the terminal stem (defined by nucleotides (nt) 1051-1056 base paired with nt 1103-1108), the 1067 stem-loop (defined by nt 1062-1076), the 1082 hairpin (defined by nt 1082-1086) and the 1095 stem-loop (defined by nt 1090-1101).

In the tertiary structure, the terminal stem stacks on the 1095 stem-loop, and the 1067 stem-loop stacks on the 1082 hairpin. Thus the four double-helical segments stack pairwise to form two extended helical subdomains. These two subdomains have irregular yet complementary shapes, so that the entire GAR RNA folds into a single compact globular domain (Figures 1b, c). The helical subdomains associate in a roughly parallel fashion, with the terminal stem packed against the 1082 hairpin, and the 1067 and 1095 stem-loops packed against each other. Bulged-out residues in the 1067 and 1095 stem-loops mediate long-range tertiary interactions between the two subdomains. The fold requires two sharp turns in the backbone at the 1056-1057 and 1086-1087 phosphodiester linkages in the center of the junction, where the chain crosses over from one helical subdomain to the other. The molecule also contains a relatively large number of well-ordered metal ions that are integral to the structure.

A ribose zipper joins the terminal stem and the 1082 hairpin

The association of the terminal stem with the 1082 hairpin occurs via their minor grooves. This rather intimate packing is stabilized primarily by a dense network of hydrogen bonds between the riboses of nucleotides A1084-A1086 and C1104-A1106 (Figure 2a). A similar structural motif has been observed in the P4-P6 domain of the group I intron, and has been referred to as a ribose zipper (Cate et al., 1996). At the center of the four-way junction, the 2′ OH of A1086 appears to be a particularly crucial component of the ribose zipper. It makes hydrogen bonds to A1103 N1 and G1056 2′ OH, and also directly ligates a crucial central cadmium ion (see below). A1086 has an unusual *syn* conformation that is necessary for the very tight packing of its sugar against the G1056-A1103 pair, and for the reverse-Watson-Crick geometry of the U1082-A1086 pair (Figure 2c). Another noteworthy feature of

the ribose zipper is a minor groove A-(G-C) triple involving nucleotides A1085, G1055 and C1104 (Figure 2c). This minor-groove triple has also been found previously in large RNA tertiary folds (Cate et al., 1996; Ferre-D'Amare et al., 1998).

Intimate association of the 1067 and 1095 stem-loops by reciprocal donation of bulges

The interaction between the 1067 and the 1095 stem-loops occurs primarily in their major grooves and is mediated largely by a reciprocal donation of highly conserved bulged-out bases. This unusually intimate major-groove packing is the primary reason for the compactness of the overall fold, and it requires substantial distortions from regular helical geometry. This portion of the structure contains a large number of tertiary interactions, some of which are novel structural motifs.

The 1095 stem donates a bulged-out base, A1088, to a pocket created by a distortion in the 1067 stem (Figure 1). A1088 forms a universally conserved reverse-Hoogsteen pair with U1060 (Figure 2c). Because of steric constraints, A1088 must be in the *syn* conformation, which together with the reverse-Hoogsteen pairing geometry requires that U1060 must be flipped over. The inversion of U1060 is in turn facilitated by bulging out of the base of U1061. This inversion-bulge, or S-turn motif, has an S-shaped backbone conformation that has been observed previously (Szewczak et al., 1993; Wimberly, 1994; Wimberly et al., 1993). The insertion of A1088 also requires that residues A1077 and U1078 are unpaired and rotated out to open up the pocket. The unpaired conformation of these residues is stabilized by three hydrogen bonds to the sugar-phosphate backbone of the 1095 stem loop at A1088 and G1089. Two of these hydrogen bonds are to the base of A1077 which explains its universal conservation.

The reciprocal donation of a bulge from the 1067 stem-loop to the 1095 stem involves

nucleotides G1071 and C1072, which form two novel interdomain base triples with the base pairs G1091-C1100 and C1092-G1099 respectively (Figures 2b, c). Within the 1095 stem loop, nucleotides G1089-(U1090-U1101) also form a triple (Figure 2c), with G1089 acting as a stacking platform for the other two triples (Figure 2b). The stacking of G1071 on G1089 is further stabilized by hydrogen bonds between the 1089 2′OH and 1071 N3, and between the 1071 2′ OH and the 1089 phosphate. These three base triples explain the sequence conservation of all these residues. The 1072-(1092-1099) triple was previously predicted and subsequently experimentally confirmed, although the geometry proposed for the triple (Conn et al., 1998) differs from that seen in the crystal structure.

The 1067 and 1095 hairpin loops

The highly conserved 1067 hairpin loop consists of two parts, a hairpin portion (U1066-A1069) that stacks on the sheared U1065-A1073 pair, and a three-nucleotide bulge (A1070-C1072) that participates in two different long-range tertiary interactions. The hairpin portion has a conformation commonly found in small hairpin loops, with a U-turn motif (Quigley and Rich, 1976) at U1066 and regular stacking of A1067-G1068-A1069. A1069 stacks on A1073, and its 2′ OH hydrogen bonds to the N3 of U1065, thereby stabilizing the location of the 1069 sugar as well as the sheared geometry of the U1065-A1073 pair. The three-nucleotide bulge has a corkscrew-like conformation in which A1070 is bulged to one side, and G1071 and C1072 are bulged into the major groove of the 1095 stem-loop. A1070 makes a novel long-range stacking interaction with U1061 which will be referred to herein as a "high-five" motif (Figure 2b), while 1071 and 1072 participate in the long-range base triples described above. The high-five motif makes several hydrogen-bonding and van der Waals interactions with the 1095 hairpin loop, thereby stabilizing the relative orientations of

the two hairpins.

The 1095 hairpin loop is also very highly conserved, and has a regular conformation stabilized by a U-turn at U1094 and a sheared G1093-A1098 pair. Part of the base of G1093 stacks over the base of C1072, so that the long-range base triples are tightly wedged between an overhang from the sheared G-A pair on one side, and the G1089-(U1090-U1101) triple on the other side. The structure of the 1095 hairpin loop is very similar to an NMR-derived structure of a small stem-loop containing the same hairpin loop sequence (Fountain et al., 1996). The structural basis for the very high sequence conservation of several of the residues in the 1095 hairpin loop (i.e. A1095, A1096 and U/C1097) is not completely clear, but it may arise from interactions with the N-terminal domain of L11 (see below) or with other components of the ribosome.

Metal ion interactions with RNA

Three cadmium ions and at least seven magnesium ions are visible in the experimental electron density map. One of the cadmium ions stabilizes the association of the two complexes in the asymmetric unit, but the other two are integral to the RNA structure, and these two sites are probably occupied by magnesium ions *in vivo*. Most of the ions mediate the close approach of phosphates in the interacting major grooves of the 1067 and 1095 stems, and five of these ions stabilize the location and conformation of the 1070-1072 bulge between the 1067 and 1095 stems (Figure 3a). A cadmium ion occupies a crucial location at the center of the four-way junction, where it makes either direct or water-mediated contacts with residues from all four double-helical stems (Figure 3b). This ion appears to stabilize both of the sharp turns at the center of the junction, i.e. the 1056-1057 and 1086-1087 turns, and thereby plays an important role in determining the overall structure of the four-way

junction.

Despite the accelerating pace of RNA structure determination, extremely little is known about RNA tertiary structure because only about five RNA folds have been determined. The crystal structure of the GAR RNA reveals an unexpectedly complex and compact fold that contains both well-known and novel structural motifs. The GAR RNA is in fact the most compact RNA structure yet reported, exposing only 138 $Å^2$ of solvent accessible surface area per nucleotide (Nicholls et al., 1991). This extreme compactness is a result of extensive tertiary interactions along the entire length of the structure, in both the major and minor grooves. The other relatively compact known RNA folds exhibit primarily minor-groove packing (e.g., the P4-P6 domain of the group I intron) or primarily major-groove packing (e.g., tRNA), and are therefore less efficiently folded. It is probable that very efficient packing of RNA will be found to be common in the ribosome.

The crystal structure explains the molecular basis for a number of important mutagenesis results. In particular, the RNA residues most sensitive to mutation are involved in tertiary interactions. For example, mutation of any of the universally conserved residues within the A1085-G1055-C1104 triple, a crucial part of the ribose zipper joining the terminal stem and the 1082 hairpin, dramatically destabilizes the RNA structure and greatly reduces the affinity for L11 (Lu and Draper, 1995). Mutation of C1072 to U within the 1072-(1092-1099) triple destroys the RNA tertiary structure, which demonstrates the energetic importance of this triple. Finally, the unusual observation that U1061A and U1061G mutants are more stable (Lu and Draper, 1994; Lu and Draper, 1995) is explained by the 1061-1070 "high five" tertiary stacking motif, since purine stacking is more stable than pyrimidine stacking.

Stabilization of the RNA tertiary structure by metal ions

The crystal structure also reveals important new information about how metal ions interact with and stabilize unusual RNA structures. Biochemical experiments suggest that the GAR RNA contains relatively high affinity binding sites for two divalent cations (Bukhman and Draper, 1997) and one K+ or NH4+ ion (Wang et al., 1993). The crystal structure reveals no fewer than seven magnesium sites and two cadmium sites, most of which stabilize the close approach of phosphates in the interacting major grooves of the 1067 and 1095 stem-loops. The metal-ion stabilization of the 1070-1072 bulge conformation is qualitatively similar – though different in detail -- to that seen in the A-rich bulge of the P4-P6 domain of the group I intron (Cate et al., 1996). The striking structural role played by the central cadmium ion suggests that this site corresponds to one of the thermodynamically important ions. While more experiments will be necessary to test this hypothesis, it is worth noting that this cadmium ion is one of the two sites in the structure that ligates a guanosine N7. Both Mn^{++} and Cd^{++} preferentially bind to guanosine N7, and it has been observed that Mn^{++} stabilizes the tertiary structure more than other divalent cations (Bukhman and Draper, 1997).

The major-groove dinucleotide platform: a generalization of the adenosine platform

The crystal structure also reveals a new variant of a known tertiary structure motif, the adenosine platform. In the structure of the P4-P6 domain, two successive adenines adopt a coplanar conformation -- an adenosine platform -- that serves as a stacking platform for a long-range tertiary interaction (Cate et al., 1996). In the GAR structure, two successive nucleotides, G1089 and U1090, adopt the same conformation seen in the adenosine platform (Figure 2C). The two bases are coplanar, with a single N2-O4 hydrogen bond between them, and they also serve as a stacking platform, for the 1071-1072 bulge involved in base triples (Figure 2B). There are, however, some differences between the GU platform seen here and

the AA platform. In the P4-P6 structure, the motif is displayed in the minor groove rather than in the major groove, as is seen here. Moreover, in the P4-P6 structure it is the 3′ adenosine upon which the long-range stacking interaction occurs, while here G1071 rests upon the 5′ residue of the motif, G1089. Finally, the tertiary stacking interaction occurs on opposite faces of the motif in the two structures. Despite these differences, the near-identity of the conformations and functions of the motifs in these two structures leads to the suggestion that the motif be referred to as a "dinucleotide platform", since it is clearly not restricted to adenosines. The few available data suggest that a GU dinucleotide platform may generally be more stable than an AA platform for major groove display. In the GAR, residues 1089 and 1090 are strictly conserved as either GU or AA, but mutation from AA to GU results in a significant stabilization of the RNA tertiary structure (Lu and Draper, 1994; Lu and Draper, 1995). The major-groove GU dinucleotide platform motif has also been found in small RNA structures lacking tertiary interactions (Szewczak et al., 1993; Wimberly et al., 1993), which suggests that in large structured RNAs, the GU dinucleotide platform may in some cases function as a pre-formed stacking platform supporting major-groove base triples.

Methylmercury as a phasing vehicle for RNA crystal structures

Surprisingly, the primary mercury site used in phasing is not near a cysteine of L11, but is located 2.4 Å from the N3 atom of U1061, consistent with a covalent mercury-uridine N3 bond. A similar, minor mercury site at U1078 is also visible in the anomalous difference Fourier map. Although most mercury adducts of pyrimidines have been obtained at the O4 or 5 positions of the base, a mercury 1-methylthymine adduct at N3 has been obtained at alkaline pH (Kosturko et al., 1974), and methylmercury salts have been shown to denature AT-rich DNA, consistent with reaction at thymine N3 (Gruenwedel and Davidson, 1966;

Gruenwedel and Davidson, 1967). Uracil is often preferred at bulge sites in RNA, so many larger RNA structures may contain solvent-accessible uracils. Therefore, methylmercury derivatization of RNA under native conditions, either prior or subsequent to crystallization, may be a generally useful method for obtaining heavy atom derivatives of RNA crystals, without the laborious incorporation of sulfur-containing ribonucleotides.

The structure of ribosomal protein L11

Ribosomal protein L11 consists of two globular domains connected by a linker region. The secondary structure and a sequence alignment of the protein are shown in Figure 4a, and the tertiary fold is shown in Figures 4b and 4c in the context of the complex. As described below, there is some flexibility between the two domains, but the linker is short and it contains two conserved prolines (73 and 74) that provide inherent rigidity. Also, the domain interface consists primarily of conserved hydrophobic residues, notably Met52, Ile53, Pro55, Pro73 and Phe77. These observations suggest that relative orientation of the two domains has not been greatly perturbed by crystal packing requirements.

The structure of the L11 N-terminal domain (NTD) has not been previously reported. It consists of two helices packed against the concave surface of a three-stranded antiparallel beta sheet, with an overall β1-α1-α2-β2-β3 topology. The N-terminal 7 residues are disordered. One of the most distinctive and conserved regions of the L11 molecule is the proline-rich helix 1, which appears to have a crucial functional role, as described below. The electron density for this helix was weak, and the register of the sequence in this helix may be in error by one residue. The average main-chain B-factor for the domain is 72 $Å^2$ (for comparison, the average B-factor of the C-terminal domain (CTD) is 24 $Å^2$), indicating rigid

body movement of the NTD within the crystal. This flexibility is consistent with the rather limited interactions seen between the NTD and other parts of the structure, and may have functional implications (see below).

The structure of the CTD is in good agreement with the previously determined NMR structures of the CTD, both in isolation (Markus et al., 1997; Xing et al., 1997) and in the context of the L11-RNA complex (Hinck et al., 1997). The domain consists of a three-helical bundle and a short parallel two-stranded β-ribbon, with an overall α3-β4-α4-α5-β5 topology. All five secondary structure elements contribute to a conserved hydrophobic core. The domain is characterized by two extended loops that are disordered in the absence of the RNA, but which have defined structures in the complex.

The RNA-protein interaction

The two domains of L11 are very unequally associated with RNA. The CTD-RNA interface covers over 1700 Å^2 of solvent accessible surface area, while the NTD-RNA interface is less than 100 Å^2. This difference is consistent with the observation that the RNA-binding affinity of the CTD is essentially the same as that of the full-length protein (Xing and Draper, 1996).

The CTD binds the minor groove of the 1067 stem (Figures 4b, c), which is bent and flatter than the minor groove of a canonical A-form double helix. The RNA-binding surface of the CTD consists of one face of helix 5, the N-terminal end of helix 3, and loops 6 and 7 that flank helix 5. Helix 5 is positioned lengthwise in the minor groove, and the flanking loops 6 and 7 extend this minor groove binding surface and also interact with the sugar-phosphate backbones on either side of the groove. A summary of the CTD-RNA interactions observed in the crystal structure (Figure 5a) emphasizes that the recognition of the RNA

minor groove by L11 involves primarily interactions between the protein backbone and the RNA 2′ OH moieties. Approximately half of the RNA-CTD hydrogen bonds involve a main-chain amide or carbonyl, and over half of the 2′OH groups in the CTD footprint are hydrogen-bonded to the protein. This preponderance of protein backbone-RNA backbone interactions indicates that overall shape complementarity between the RNA and protein must be an important determinant of specificity.

Although binding appears to depend less on electrostatic interactions than on shape complementarity, there are a number of important salt bridges between basic sidechains and phosphate groups: lysines 93, 126 and 133 and Arg94 interact with one side of the minor groove, and lysines 80, 87 and 112 with the other side. In the former group, the sidechains are splayed away from protein, and the hydrophobic part of the sidechain contributes to surface complementarity with the RNA. Sidechains at the N-terminus of α5 and within loop 7 make particularly intimate contact with the RNA, notably Ile127 and Asn117. Asn117 points directly into the minor groove making a number of hydrogen bonding interactions, and is one of the few sidechains that formally "reads" the local RNA sequence. Two of the most important recognition elements in the RNA are the universally conserved long-range pair U1060-A1088 and the surrounding RNA internal loop that distorts to accommodate the insertion of A1088. Significantly, the RNA footprint of helix 5 encompasses this entire region of distorted RNA. The importance of the U1060-A1088 pair for L11 specificity is shown by the extremely high conservation of Gly130 and Thr131 to which these bases are hydrogen-bonded (Figure 5b).

The NTD bridges the interface between the 1067 and 1095 stem-loops, and it makes only a few specific interactions with the RNA (Figure 4). Although its association with RNA

is somewhat tenuous, which might be a result of its binding mode having been altered by crystal packing requirements, the high sequence conservation of the NTD residues interacting with RNA suggests that the binding mode observed in the crystal structure is relevant to the structure of the complex in solution. Moreover, as described above, the structure of the NTD-CTD interface also suggests that the orientation of the NTD has not been greatly perturbed by crystal packing. The NTD residues interacting with RNA include Lys10, Gln12, Gln30 and Lys71. Lys10 makes both main-chain and side-chain interactions with the RNA, and Gln 30 probably interacts specifically with A1095. There is also electron density interacting with the Watson-Crick face of C1097, but it is not clear whether this density arises from the NTD; examination of an anomalous difference Fourier map reveals that some of this density must correspond to a mercury or cadmium site. Finally, although the proline-rich sequence in helix 1 is surface-exposed, highly conserved, and in the correct orientation for possible interactions with factors or antibiotics, it is close to but not in direct contact with RNA.

The thiostrepton/micrococcin binding site

A1067 and A1095, at the ends of their respective stem-loops, have both been implicated in the binding of the antibiotics thiostrepton and micrococcin. Modification of A1067 by 2′-O methylation (Cundliffe and Thompson, 1979; Thompson et al., 1982) or transversion mutations at either site (Rosendahl and Douthwaite, 1994) confers thiostrepton resistance. It has also been shown that thiostrepton affects the reactivity of both A1067 and A1095, suggesting that these two sites are close together (Rosendahl and Douthwaite, 1994) as indeed they are in the crystal structure. As for the role of L11 in antibiotic binding, it is known that L11 is required for high affinity binding of thiostrepton to the RNA, and that binding of L11 and thiostrepton to the RNA is cooperative. Thiostrepton has a much weaker

affinity for the RNA alone (Kd = 0.4 μM), and it does not bind isolated L11 (Thompson et al., 1979). Two sites within the NTD of the protein have been implicated in this interaction: the mutations Pro22Ser and Pro22Thr confer thiostrepton resistance, while the antibiotic protects Tyr61 (Tyr62 in *E. coli*) in protein footprinting experiments (Porse et al., 1998). Recently, mutations that confer resistance to micrococcin have also been mapped to the NTD of L11 between residues 22 and 32 (Porse et al., 1999). All of these sites are located on a small surface of the NTD, near A1067 and A1095 on the RNA (Figure 6). A prominent feature of this surface is the distinctive and highly conserved proline-rich helix, while Tyr61 is over 20 Å distant. The clustering of these sites of antibiotic resistance mutations, together with the cooperative binding data, strongly suggest that the antibiotics bind to the cleft between the RNA and the proline-rich helix 1 of the NTD.

The structure of the C-terminal domain (CTD) was previously determined by NMR in both the free (Markus et al., 1997; Xing et al., 1997) and RNA-bound (Hinck et al., 1997) forms. Our crystal structure of the CTD is similar to that of the RNA-bound form determined by NMR, except for the conformation of the large RNA-binding loop 6 which is poorly determined in the NMR studies (Hinck et al., 1997). The mean Cα root mean square difference (RMSD) for the crystal structure vs. NMR ensemble is 2.7 Å overall, or 1.6 Å when residues 86-97 of loop 6 are excluded. For comparison, the mean RMSD within the ensemble of NMR structures is 2.3 Å for main chain atoms.

Many ribosomal proteins show structural similarities to families of DNA- and RNA-binding proteins (Ramakrishnan and White, 1998). It was noted from the NMR structure that the CTD of L11 has a homeodomain-like fold (Markus et al., 1997; Xing et al., 1997), and further NMR studies on the complex suggested that the CTD uses the typical homeodomain

helix to bind RNA (Hinck et al., 1997). Although the crystal structure reveals that this helix is indeed intimately associated with the RNA, its interaction does not bear any similarity to the base-specific recognition of a major groove by the homeodomains. Regarding the NTD, its overall $\alpha + \beta$ fold is similar to that seen in many other RNA-binding proteins (Ramakrishnan and White, 1998), but its β-α-α-β-β topology has not yet been observed in an RNA-binding protein.

RNA-protein interaction

The L11-GAR RNA interaction has been probed by biochemical and NMR methods, and the crystal structure is in good agreement with the results of these studies, including a rather weak interaction between the RNA and the NTD. The RNA surface covered by the CTD corresponds fairly well to the residues protected by the binding of full-length L11 as shown by hydroxyl radical footprinting experiments (Rosendahl and Douthwaite, 1993). The RNA-binding surface of the CTD has been mapped by NMR chemical shift changes and relaxation studies (Hinck et al., 1997), and again the agreement with the crystal structure is excellent. The observation that L11 recognizes the RNA primarily by shape complementarity rather than by a sidechain-base reading of the RNA sequence is not surprising considering that the interaction occurs primarily via the minor groove. The interaction agrees with the prediction that relatively few highly conserved CTD residues would make specific sidechain contacts with RNA (Xing et al., 1997). However, the related prediction that RNA binding by the CTD would not involve extensive recognition of the RNA bases is incorrect, as most of the base pairs are recognized by either hydrogen bonding or hydrophobic interactions. However, most of these hydrogen bonds occur via main chain amides or carbonyls, rather than side chains. Finally, it is worth noting that L11 does not directly recognize the bulged-

out nucleotides, which have previously been proposed as specificity determinants in ribosomal RNA-protein complexes.

Biochemical experiments have shown that L11 stabilizes the tertiary structure of the RNA, and that this is a property of the CTD (Draper and Xing, 1995; Xing and Draper, 1995). Since nearly all of the direct RNA-protein contacts within the complex are to the 1067 stem, the resulting stabilization of the RNA tertiary structure appears to be indirect. The binding of one face of helix 5 with both strands of the 1067 stem is extensive and universally conserved, and this interaction must be particularly important for stabilization of the RNA tertiary structure. Consistent with a crucial role in RNA binding, helix 5 contains most of the mutation sites that have the greatest adverse effect on binding affinity (T131V, G130A, K126A, and S134A) (Xing et al., 1997). As for the RNA-binding loops 6 and 7, both are disordered when not bound to RNA (Markus et al., 1997), but they are highly ordered in the complex, and their conformations match the groove surface perfectly. The loops contain conserved structural features, which are important in the complex and which may predispose them for RNA-binding. Although it makes many interactions with RNA and contains the other two sites most sensitive to mutation (G88P and P92G), the longer RNA-binding loop 6 is relatively poorly conserved between kingdoms, with the bacterial and archaeal loops differing significantly from the eukaryotic loops (Figure 4A). This variability in the protein sequence correlates with variability between phylogenetic kingdoms in the base-pairing of the upper portion of the 1067 stem.

The NTD as a molecular switch

Prior to these structural studies, the molecular basis for cooperative binding within the RNA-L11-thiostrepton ternary complex was unknown. The crystal structure now provides a

very straightforward explanation that also rationalizes the particular importance of the L11 NTD. The model also provides insights into how the GAR might function as a molecular switch.

The putative thiostrepton/micrococcin binding site is centered on a small gap between helix 1 of the NTD and the 1067/1095 region of the RNA (Figure 6). The antibiotics are proposed to bind within this gap, possibly enlarging it somewhat, making specific interactions with the RNA on one side and further interactions with the NTD on the other side. In the absence of the NTD, the antibiotic's binding affinity would be greatly compromised, thus explaining the importance of the NTD for antibiotic binding (Xing and Draper, 1996). An alternative proposal, that thiostrepton binds directly only to the RNA and that this RNA conformation requires the presence of the NTD, is unlikely because the NTD does not appear to stabilize the RNA tertiary structure significantly, and because the NTD sites of resistance mutations are not in contact with the RNA. In a model that better accounts for previously known data and agrees with the crystal structure reported herein, the mechanism for the resistance to thiostrepton in Pro22 mutants would be a disruption of direct thiostrepton-Pro22 interaction. A similar mechanism must hold true for the micrococcin sites given the more recent data (Porse et al., 1999). Regarding the details of the interaction of thiostrepton and micrococcin with RNA, we note that these antibiotics contain an array of thiazole rings that resembles the array of prolines in the conserved proline-rich NTD helix.

The data disclosed herein suggests a potential mechanism of thiostrepton inhibition of factor-dependent GTPase activity involves restriction or "trapping" of one of the many conformational states that must occur during elongation (Cundliffe, 1986) by the antibiotic. In their analysis of the effects of the Pro22Ser and Pro22Thr mutations, Porse *et al.* (1998)

suggest that thiostrepton binding may affect the ability of the L11 NTD to undergo a conformational change, an idea which merits closer examination in light of the crystal structure. In the structure, the CTD is rather firmly anchored to one of the two RNA subdomains, while the NTD is somewhat tenuously bound across the RNA subdomain-subdomain interface. Even in the absence of other data, this overall architecture suggests that the NTD may function as a molecular switch that reversibly associates with the GAR RNA during the elongation cycle. In light of the other data -- in particular the cooperative binding of thiostrepton and full-length L11 to RNA, and the clustering of antibiotic resistance mutations to the cleft defined by A1067/A1095 and the proline-rich NTD helix -- it appears even more likely that the NTD functions as a molecular switch, and that the thiazole antibiotics work by binding to the NTD-RNA interface, thereby preventing the NTD from switching between RNA-bound and RNA-free states. It is possible that the switch is coupled to, or triggered by, the binding of elongation factors. It is important to note that the NTD itself cannot provide the actual GTPase enhancing activity since L11 is not required for viability in *E. coli* (Stöffler et al., 1980). Therefore, the switch appears likely to function by controlling either the accessibility or the conformation of the GAR RNA.

This switch hypothesis could also explain why EF-Tu and IF2 do not footprint the 1067/1095 region of RNA, while EF-G does, even though all these factors interact with the sarcin/ricin loop (Moazed et al., 1988). The sarcin/ricin loop is known to bind to a nearby (Wilson and Noller, 1998) but distinct (Munishkin and Wool, 1997) site on EF-G. The EF-Tu-tRNA complex is similar in structure to EF-G, and the similarity is thought to be a case of molecular mimicry, with the factors binding to the same general region of the ribosome (Nissen et al., 1995). Thus the footprinting differences could be explained if EF-Tu and IF2

recognize a different conformation of the switch than EF-G does. This reasoning suggests that the two conformations of the GAR molecular switch correspond to different functional states of the ribosome.

The structure features a complex and very compact RNA fold stabilized by many bound metal ions, by a dense network of RNA tertiary interactions, and by extensive interactions with the protein. The overall architecture of the complex suggests that the N-terminal domain functions as a molecular switch, either by facilitating changes in the tertiary structure of the GAR RNA, or by controlling access to the RNA. Thiostrepton and micrococcin are proposed to bind to the NTD-RNA interface, thus locking the switch and disrupting GAR function.

Uses of the Crystal Structure Coordinates of the L11/GAR Complex

One approach enabled by the X-ray crystal structure disclosed herein is the use of the crystal coordinates for the rational design of GAR activity modulators, either de novo or by modification of known compounds. The modulators identified through use of the crystal structure coordinates will be useful for altering the rate of bacterial protein synthesis, and thereby the rate of bacterial cell growth. It is expected that, for example, an inhibitor of GAR function will inhibit bacterial cell proliferation, and will thus potentially have immediate medical usefulness.

One of skill in the art may use the structure data disclosed herein and the

computer-modeling techniques described herein to develop models of target domains also selected through analysis of the crystal structure data (see below). These models can be used to provide a detailed analysis of the binding surfaces, including factors such as van der Waals contacts, electrostatic interactions and hydrogen-bonding opportunities. This information is then used with computer simulation techniques to map the favorable interaction positions for functional groups such as protons, hydroxyl groups, amine groups, divalent cations, aromatic and aliphatic functional groups, acetamide, methanol, etc. These groups may then be designed into a synthetic ligand.

The L11/GAR structure coordinates may be used to screen computationally small molecule data bases for chemical entities or compounds that may bind in whole, or in part, to the L11/GAR, to GAR, or to Lll.

In addition, because the L11/GAR RNA complex may be crystallized in more than one crystal form (e.g, as a co-crystal with another factor, such as EF-G), the structure coordinates of the L11/GAR RNA, or portions thereof, as provided by this invention are useful to solve the structure of those other crystal forms of the L11/GAR RNA complex. One method that may be employed for this purpose is molecular replacement. In this method, the unknown crystal structure (i.e., that of the co-complex) may be determined using the L11/GAR complex structure coordinates of this invention as provided in Fig. 7. This method will provide an accurate structural form for the unknown crystal more quickly and efficiently than attempting to determine such information from first principles.

In addition, in accordance with this invention, the L11/GAR complex may be crystallized in co-complex with known GAR inhibitors (e.g., thiostrepton, micrococcin). The crystal structures of such complexes may then be solved by molecular replacement and compared with that of inhibitor-free L11/GAR complex. Critical sites for interaction of the

known inhibitor with the L11/GAR may thus be identified at high resoultion. This information provides an additional tool for determining the most efficient binding interactions, for example, increased hydrophobic interactions, between L11/GAR and a chemical entity or compound.

All of the complexes referred to above may be studied using well-known X-ray diffraction techniques and may be refined versus 2-3 Å resolution X-ray data to an R value of about 0.20 or less using computer software, such as X-PLOR (Yale University, ©1992, distributed by Molecular Simulations, Inc.). See, e.g., Blundel & Johnson, supra; Methods in Enzymology, 1985, vol. 114 & 115, H. W. Wyckoff et al., eds., Academic Press. The crystallographic information disclosed herein may thus be used to optimize known classes of L11/GAR inhibitors or activators.

Importantly, the X-ray crystal data disclosed herein also allows the design and synthesis of novel classes of L11/GAR inhibitors or activators (i.e., modulators). The design of compounds that bind to or modulate L11/GAR function according to this invention generally involves consideration of several factors. In particular, the compound must be capable of physically and structurally associating with L11/GAR. Non-covalent molecular interactions important in the functional association of L11/GAR with its accessory factors include hydrogen bonding, van der Waals, electrostatic and hydrophobic interactions.

It is recognized that although certain portions of the compound will not directly participate in this association with the L11/GAR, those portions may still influence the overall conformation of the molecule. This, in turn, may have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity or compound in relation to all or a portion of the binding site, or the spacing between functional groups of a compound comprising several chemical

entities that directly interact with L11/GAR.

The potential modulating or binding effect of a chemical compound on the L11/GAR may be analyzed prior to its actual synthesis and testing by the use of computer modelling techniques. If the theoretical structure of the given compound suggests insufficient interaction and association between it and the L11/GAR, synthesis and testing of the compound is obviated. However, if computer modelling indicates a strong interaction, the molecule may then be synthesized and tested for its ability to bind to the L11/GAR domain and to inhibit using the assays described herein. In this manner, synthesis of inoperative compounds may be avoided.

A modulating or binding compound of the L11/GAR may be computationally evaluated and designed by means of a series of steps in which chemical entities or fragments are screened and selected for their ability to associate with the individual binding targets on the L11/GAR.

One skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with L11/GAR and more particularly with the individual binding domains comprising the L11/GAR active sites. This process may begin by visual inspection of, for example, the active site on the computer screen based on the L11/GAR RNA coordinates in Fig.7. Selected fragments or chemical entities may then be positioned in a variety of orientations, or "docked", within an individual binding target site of the L11/GAR as defined herein from analysis of the crystal structure data. Docking may be accomplished using software such as Quanta (Molecular Simulations, Inc., San Diego, CA) and Sybyl (Tripos, Inc., St. Louis, MO) followed by energy minimization and molecular dynamics with standard molecular mechanics forcefields, such as CHARMM (Molecular Simulations, Inc., San Diego, CA) and AMBER (University of California at San Francisco).

Specialized computer programs may also assist in the process of selecting fragments or chemical entities. These include:

1. GRID (Goodford, P. J., "A Computational Procedure for Determining Energetically Favorable
Binding Sites on Biologically Important Macromolecules", J. Med. Chem., 28, pp. 849-857 (1985)). GRID is available from Oxford University, Oxford, UK.

2. MCSS (Miranker, A. and M. Karplus, "Functionality Maps of Binding Sites: A Multiple Copy
Simultaneous Search Method." Proteins: Structure. Function and Genetics, 11, pp. 29-34 (1991)).
MCSS is available from Molecular Simulations, San Diego, CA.

3. AUTODOCK (Goodseil, D. S. and A. J. Olsen, "Automated Docking of Substrates to Proteins
by Simulated Annealing", Proteins: Structure. Function, and Genetics, 8, pp. 195-202 (1990)).
AUTODOCK is available from Scripps Research Institute, La Jolla, CA.

4. DOCK (Kuntz, I. D. et al., "A Geometric Approach to Macromolecule-Ligand Interactions", J.
Mol. Biol., 161, pp. 269-288 (1982)). DOCK is available from University of California, San Francisco, CA.

5. CERIUS II (available from Molecular Simulations, Inc., San Diego, CA).

6. Flexx (Rarey et al., 1996, J. Mol. Biol. 261: 470-489).

Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound or modulator. Assembly may proceed by visual inspection

of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of the L11/GAR. This would be followed by manual model building using software such as Quanta or Sybyl.

Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include:

1. CAVEAT (Bartlett, P. A. et al, "CAVEAT: A Program to Facilitate the Structure-Derived Design of Biologically Active Molecules". In "Molecular Recognition in Chemical and Biological Problems", Special Pub., Royal Chem. Soc., 78, pp. 182-196 (1989)). CAVEAT is available from the University of California, Berkeley, CA.

2. 3D Database systems such as MACCS-3D (MDL Information Systems, San Leandro, CA). This area is reviewed in Martin, Y. C., "3D Database Searching in Drug Design", J. Med. Chem.,

35, pp. 2145-2154 (1992)).

3. HOOK (available from Molecular Simulations Inc., San Diego, CA.).

Instead of proceeding to build an L11/GAR modulator in a step-wise fashion one fragment or chemical entity at a time as described above, modulatory L11/GAR binding compounds may be designed as a whole or "de novo" using either an empty active site or optionally including some portion(s) of a known inhibitor(s). These methods include:

1. LUDI (Bohm, H.-J., "The Computer Program LUDI: A New Method for the De Novo Design

of Enzyme Inhibitors", J. Comp. Aid. Molec. Design, 6, pp. 61-78 (1992)). LUDI is available from Molecular Simulations, Inc., San Diego, CA.

2. LEGEND (Nishibata, Y. and A. Itai, Tetrahedron, 47, p. 8985 (1991)). LEGEND is available

from Molecular Simulations, San Diego, CA.

3. LeapFrog (available from Tripos Associates, St. Louis, Mo.).

Other molecular modelling techniques may also be employed in accordance with this invention. See, e.g., Cohen, N. C. et al., "Molecular Modeling Software and Methods for Medicinal Chemistry", J. Med. Chem., 33, pp. 883-894 (1990). See also, Navia, M. A. and M. A. Murcko, "The Use of Structural Information in Drug Design", Current Opinions in Structural Biology, 2, pp. 202-210 (1992); Hubbard, "Can Drugs Be Designed?", Curr. Opin. Biotechnol., 8, pp. 696-700 (1997); and Afshar et al., "Structure-Based and Combinatorial Search for New RNA-Binding Drugs", Curr. Opin. Biotechnol., 10, pp.59-63 (1999).

Once a compound has been designed or selected by the above methods, the efficiency with which that compound may bind to L11/GAR may be tested and optimized by computational evaluation. For example, a compound may be optimized so that in its bound state it would preferably lack repulsive electrostatic interaction with the target site. Such non-complementary (e.g., electrostatic) interactions include repulsive charge-charge, dipole-dipole and charge-dipole interactions. Specifically, the sum of all electrostatic interactions between the modulator and the enzyme when the modulator is bound to L11/GAR preferably make a neutral or favorable contribution to the enthalpy of binding.

Specific computer software is available in the art to evaluate compound deformation energy and electrostatic interaction. Examples of programs designed for such uses include: Gaussian 92, revision C [M. J. Frisch, Gaussian, Inc., Pittsburgh, Pa. ©1992]; AMBER,

version 4.0 [P. A. Kollman, University of California at San Francisco,©1994]; QUANTA/CHARMM [Molecular Simulations, Inc., San Diego, CA.©.1994]; and Insight II/Discover (Biosysm Technologies Inc., San Diego, CA. ©1994). These programs may be implemented, for instance, using a Silicon Graphics workstation, 02-R10000 or IBM RISC/6000 workstation model 550. Other hardware systems and software packages will be known to those skilled in the art.

Once an L11/GAR-binding compound has been optimally selected or designed, as described above, substitutions may then be made in some of its atoms or side groups in order to improve or modify its binding properties. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. It should, of course, be understood that components known in the art to alter conformation should be avoided. Such substituted chemical compounds may then be analyzed for efficiency of fit to L11/GAR by the same computer methods described in detail, above.

Targets for Modification of L11/GAR Function

The X-ray crystal structure co-ordinates disclosed herein may be used to define structural features of the L11/GAR which represent targets for inhibition or activation of the GTPase activity of the ribosome. The following regions of the L11/GAR, defined by the X-ray co-ordinate data, represent particularly useful targets for the development of inhibitory or activating compounds.

1. L11 N terminus:GAR RNA interface.

The putative site for binding of the antibiotics thiostrepton and micrococcin to the

GAR is between the N terminus of L11 and the interface between the 1067 and 1095 stem loops of the GAR RNA. The structural data as disclosed in Table II and described herein above suggest that the N terminal lobe of L11 behaves as a rigid body that flexes about the so-called "tether sequence" between the C terminal and N terminal lobes of the protein. Therefore, the binding pocket is not limited to those residues at the interface of the L11 N terminus and the GAR RNA that are in direct contact. The binding pocket can include all of the following:

A) all exposed residues from the L11 N terminus;

B) all exposed residues from the GAR RNA that are on its L11 binding surface, including A1070, U1061, A1095, A1096, C1097, and A1098;

C) L11 amino acid residues that are in direct contact with the GAR RNA, including K10, Q12, Q30 and K71;

D) L11 amino acid residues from the helical region between P20 and H31; and

E) the L11 β sheet between Q8 and P14, and neighboring I53.

Computer simulation techniques may be used to determine which parameters of the binding pocket may be exploited in designing or screening compounds that interact with the binding pocket. Such techniques allow for the construction of structural models that can then be used in designing inhibitory/activating compounds targeted to the L11/GAR binding pocket. These techniques may involve any of the software packages described above or known in the art, and include:

A) Interactive movement of the L11 N terminus as a rigid body with concurrent geometry optimization, using, for example, Quanta.

B) Molecular dynamics simulation of the GAR RNA-L11 complex using. For

example, CHARMM and/or AMBER.

C) Normal mode dynamics simulation of the GAR RNA-L11 complex using, for example, CHARMM.

D) Molecular docking of thiostrepton and/or micrococcin to the models of the binding pocket.

2. The L11 flexible tether or the flexible tether:GAR RNA interface.

The flexible tether domain of L11 and the GAR RNA surfaces that the tether domain interacts with are defined by the crystal structure coordinates disclosed in Table II and discussed herein above. The X-ray crystal data suggest that the L11 N terminus may act as a molecular switch that triggers the GTPase activity. It is thought that thiostrepton and micrococcin act by modifying the interaction between the L11 N terminus and the GAR RNA. Therefore, the region tethering the N terminal and C terminal lobes of L11, (i.e., amino acids K71 through A75) represent a target for the development of compounds that inhibit or activate GAR function, as does the domain comprising the interface of the tether region with GAR RNA residues. The GAR RNA domain interacting with the tether includes U1061, the backbone of U1060, and G1059. Any molecule that could modify the relative positioning of the Lll NTD and CTD may disrupt the funtion of the molecular switch and thereby modulate the function of the GAR. For example, this could be performed by a molecule interacting with the Lll tether domain and/or the GAR in close contact with the tether. Any molecule that could interact with both the C terminal and N terminal lobes of L11 and stabilize one orientation of the lobes relative to the alternate orientation may disrupt the function of the molecular switch and thereby disrupt the function of the GAR.

Computer simulation techniques similar to those described above for modeling the

L11 N terminus:GAR RNA interface may be used to determine which parameters of the 4 way junction and Cd^{++} coordination site may be exploited in designing or screening compounds that interact with or disrupt the junction/Cd^{++} coordination site and/or modify the activity of the GTPase.

3. The GAR RNA:EF-G interface.

The interaction of translational elongation factor EF-G with the ribosome has been mapped by directed hydroxyl radical probing (Wilson & Noller, 1998, Cell 92: 131-139). This approach indicated that GAR RNA residues in the region of A1070 and in the region of C1100 are involved in the binding of EF-G. A1070 is included in the GAR RNA:L11 N terminal interface discussed as a target above, but is nonetheless of interest in approaches aimed at disrupting or modifying EF-G binding.

The crystal structure coordinates disclosed in Table II and discussed herein above define the structure of the GAR RNA at C1100, and the RNA bases and L11 amino acid residues around it. This structure defines a novel target for the design and/or selection of molecules that can disrupt the GAR RNA:EF-G interaction.

Computer simulation techniques similar to those described above for modeling the L11 NTD: GAR RNA interface may be used to determine which parameters of the binding pocket may be exploited in designing or screening compounds that modify the relative positioning of Lll NTD and CTD and modify the activity of the GTPase.

4. RNA Folding/Stability.

The X-ray crystal structure coordinates disclosed in Table II and discussed herein above define the structure of a novel "4 way junction" fold in the ribosomal RNA in the L11/GARcomplex. The data further reveal the importance of a Cd^{++} ion that occupies the center of the four way junction between bases 1056-1057 and 1086-1087. Because a ligand

that can modify the folding of the RNA would be predicted to disrupt or otherwise modify the GTPase activity, this folded RNA structure represents a strong target for development of inhibitors or activators of the GTPase. Because the Cd^{++} ion likely stabilizes the unusual RNA fold, the region defined by those amino acid and RNA residues interacting with the Cd^{++} ion is particularly attractive as a target.

5. The L11 C terminus:GAR RNA interface.

The domain comprising the interaction surface of the C terminal lobe of L11 and the GAR RNA is defined by the crystal structure data disclosed in Table II (X-ray co-ord's) and is described herein above. The crystal data indicate that the C terminus of L11 interacts very tightly with the GAR RNA. As such, the interaction may be difficult to disrupt. Computer simulation techniques similar to those described above for modeling the L11 N terminus:GAR RNA interface may be used to determine which parameters of the binding pocket may be exploited in designing or screening compounds that interact with the C terminal L11: GAR RNA interface domain and/or modify the activity of the GTPase.

The analysis of the various targets made possible by the crystal structure coordinate data disclosed herein, including the GAR RNA:L11 interface, the GAR RNA:L11: Micrococcin interface, the L11 N terminus:L11 C terminus interface (with or without GAR RNA), the GAR RNA:EF-G interface, and the GAR RNA:L11:EF-G interface, may be used to define specific features (e.g., a pattern of hydrogen bond donors and acceptors, a hydrophobic patch, etc.) of these targets. These features in turn define a three dimensional "pharmacophore" pattern. This pattern can then be used to screen virtual libraries of existing compounds, such as the Available Chemical Directory (MDL, Inc.) for compounds exhibiting the desired combination of chemical entities. In this screening, the quality of fit of such entities or compounds to the target site may be judged by a scoring fuction. The scoring

function can account for shape complementarity (Katchalski-Katzir et al., 1992, Proc. Natl. Acad. Sci. USA, 89, pp.2195-2199.), estimated interaction energy (Meng et al., 1992, J.Comp. Chem., 13, pp. 505-524), surface accessibility, or a combination of these (see for example, Bohm, 1994, J. Comp. Aided Mol. Design, pp.243-256). A program such as Catalyst (MSI) can perform this task. Libraries of compounds can also be screened virtually using the coordinates of the targets and molecular docking programs such as DOCK (UCSF) or FLEXX.

Once one or more compounds have been identified as potential ligands using any of the methods described above, they may be screened for biological activity.

A variety of assays can be used to evaluate the activity of compounds designed to inhbit the activity of the L11/GAR. These include, but are not limited to: inhibition of bacterial growth,

inhibition of in vitro protein synthesis using messenger RNA as a template, inhibition of the elongation phase of in vitro protein synthesis using polyU as a template, inhibition of GTP hydrolysis mediated by EF-G as described by Pestka (1970) and Rodnina et al. (1997); activation of GTP hydrolysis mediated by EF-G as described by Cundliffe and Thompson (1981). Binding of EF-G to both the L11/GAR complex and to the sarcin/ricin domain can be measured as described by Munishkin and Wool (1997, Proc. Natl. Acad. Sci. USA 94, 12280-12284; "The ribosome in pieces: Binding of elongation factor EF-G to oligoribonucleotides that mimic the sarcin/ricin and thiostrepton domains of 23S ribosomal RNA").

In addition, compound interaction with the L11/GAR complex can be evaluated by direct binding assays. Filter binding assays that measure the ability of thiostrepton to cause retention of radiolabelled GAR RNA to nitrocellulose filters have been described by

GuhaThakurta and Draper (1999; Biochemistry, 38, 3633-3640 "Protein-RNA sequence covariation in a ribosomal protein-rRNA complex"). As revealed herein, these assays can be modified to evaluate small molecules that competitively inhibit the binding of thiostrepton and/or micrococcin to the L11/GAR complex or to GAR. For molecules that do not themselves cause filter retention,

the RNA may be labelled. For molecules that do cause filter retention, the RNA and/ or RNA-protein complex can be immobilised on a solid support and the binding of radiolabelled thiostrepton or other known L11/GAR binding compound can be measured. Thiostrepton or micrococcin can be labelled metabolically by incorporation of 35S, 3H or 14C labelled precursors, or post-synthetically by modifcation of the molecule with radiolablled precursors. In addition thiostrepton or micrococcin can be labelled with another detectable group, including, but not limited to, fluorescent and luminescent groups.

Displacement assays can also be performed by using as reporter molecules any labelled molecule that binds to the L11/GAR complex or GAR RNA with an affinity of 50 uM or less. Suitable reporters include, but are not limited to, oligonucleotides, peptides and oligonucleotide-peptide conjugates.

Libraries for Screening According to the Invention.

Inhibitors and/or activators identified according to the methods of the invention may be provided from libraries of compounds available from a number of sources or may be derived by combinatorial chemistry approaches known in the art. Such libraries include but are not limited to the available Chemical Directory, Maybridge, and natural product collections.

Compounds identified as ligands using the methods described herein may be further optimized to improve binding activity. Using the docked models of the known ligands

thiostrepton and micrococcin, it is possible to identify structures of the ligand that may be altered to improve binding affinity. Similarly, features of a ligand that are identified as unimportant for binding may be excluded to reduce the molecular weight of the ligand.

EXAMPLES

In order that the invention described herein may be more fully understood, the following examples are set forth. It should be understood that these examples are for illustrative purposes only and are not to be construed as limiting this invention in any manner.

EXAMPLE 1: Preparation and Analysis of L11/GAR RNA Crystal.

A. Sample Preparation

The gene for *T. maritima* ribosomal protein L11 was cloned and overexpressed in *E. coli* using the T7-based expression system (Studier et al., 1990). The protein was purified by a combination of cation-exchange, hydroxylapatite and size-exclusion chromatography as reported for the purification of ribosomal protein S7 (Wimberly et al., 1997). For cocrystallization with RNA, the protein was dialysed into a buffer A containing 0.1 M KCl, 5 mM Na-cacodylate pH 6.0, 0.1 mM Na2EDTA, 1 mM DTT. A fragment of RNA corresponding to nucleotides 1111-1168 of *T. maritima* 23S rRNA was synthesized by *in vitro* run-off transcription from a linearized plasmid using T7 RNA polymerase. The plasmid contained the following elements: a T7 promoter, a self-cleaving hammerhead ribozyme to generate a homogeneous RNA 5′ end (Price et al., 1995), a template for the target RNA sequence, and a Pst I site used for plasmid linearization. RNA was purified on denaturing polyacrylamide slab gels, eluted, concentrated by ethanol precipitation, and dialyzed into

buffer A. The RNA was reannealed by heating to 90 °C and slow cooling. L11 protein was added to yield a 1:1 RNA:protein mixture, which was concentrated to 0.15 mM in each component for crystallization experiments.

B. Crystallization and Structure Determination

Crystals of the complex were obtained at 4 °C using the hanging drop technique. The equimolar mixture of L11 and RNA in dialysis buffer A was mixed with an equal volume of well solution (25% glycerol, 15% PEG 4000, 0.2 M KCl, 50 mM MgCl2, 20 mM CdCl2, 1 mM DTT, 50 mM Tris pH 7.5 at 22°C). The crystals were in the space group P212121, with cell dimensions of a = 63.9 Å, b = 84.3 Å and c = 155.5 Å, and diffracted to better than 2.6 Å resolution using a synchrotron source. Diffraction data were collected under cryogenic conditions, and the crystals were flash-frozen by plunging into liquid nitrogen. For mercury derivatization, crystals were soaked for 24 hours in the well solution containing 1 mM CH3HgNO3 but lacking DTT. Efforts to obtain cocrystals of RNA with selenomethione-substituted L11 were unsuccessful, apparently because the preparation of selenomethionyl L11 used was at least partly misfolded.

The structure was solved using a multiwavelength anomalous diffraction (MAD) experiment (Hendrickson, 1991) on the methylmercury derivative. Straightforward isomorphous replacement was not possible because the derivative is not isomorphous with native crystals. Because the mercury LIII edge does not have a significant white line, data were collected at just two wavelengths, the inflection point of the mercury edge at 1.01 Å and a remote wavelength at 0.98 Å. This remote wavelength is near the maximum f'' for accurate measurement of anomalous differences, and is also sufficiently remote from the inflection point to give useful isomorphous differences. Data were collected from a single flash-cooled

crystal at beamline X12-C of the NSLS. To optimize measurement of anomalous differences, we used the inverse beam method in which pairs of sweeps separated by 180 degrees in were collected every 30 degrees. The data were integrated and scaled using the HKL suite of programs (Otwinowski and Minor, 1997).

Phasing was done by treating MAD as a special case of MIR (Ramakrishnan and Biou, 1997; Ramakrishnan et al., 1993). Local scaling of the data, determination of initial heavy atom sites, and initial phasing was done using the program SOLVE (Terwilliger and Berendzen, 1999). Subsequent phasing was done using the program SHARP (de la Fortelle and Bricogne, 1997). A significant improvement in phasing was obtained by including several well-ordered cadmium sites in a final round of SHARP heavy atom refinement. Each round of phasing was followed by density modification with Solomon (Abrahams and Leslie, 1996). The unaveraged, solvent-flattened map revealed virtually unbroken main-chain density for the RNA and the L11 C-terminal domains of both complexes in the asymmetric unit, which were easily built using the program O (Jones and Kjeldgaard, 1997). Twofold non-crystallographic symmetry (NCS) averaging followed by solvent flattening was then carried out using NCS and solvent masks based on the RNA and C-terminal domain coordinates. The resulting map was of high quality and revealed a few minor building errors, but the L11 N-terminal domain density was still of insufficient quality to permit unambiguous fitting. Interpretation of the density for the entire L11 N-terminal domain was possible only from iterative rounds of refinement and $2F_o$-F_c maps. The final model was refined to an Rfree of 27 % using the program X-PLOR (Brünger, 1988) using standard parameters for protein (Engh and Huber, 1991) and nucleic acid (Parkinson et al., 1996) structure refinement. Magnesium and cadmium ions were distinguished by inspection of an anomalous difference Fourier map.

Magnesium ions were distinguished from ordered waters by inspection of $2F_o$-F_c maps, in which an octahedral coordination of magnesium by water and RNA ligands was often visible. A Ramachandran plot of the protein revealed only three outliers, Lys93 in the C-terminal domain, which clearly has a positive phi angle in the original experimental map, and Ala21 and Val24 in the N-terminal domain, for which the side chains are very poorly defined. Details of the data collection, phasing and refinement are shown in Table I.

EXAMPLE 2. Use of the Ribosomal Protein L11/GAR Crystal Structure Coordinates to Design a Modulator of GAR Activity.

Example 1 illustrates the methods involved in generating a structure of the L11/GAR RNA complex at atomic resolution. The crystal structure data make clear, for example, that the N terminus of L11 can move within the context of the L11/GAR. Because the crystal structure data, in conjunction with available biochemical data, point to a molecular switch mechanism whereby the relative position of the L11 N terminal lobe determines the activity of the GAR, it is of interest to select or design compounds that can effect restriction of modification of this movement.

1. Modeling the movement and interactions of the L11 N terminal lobe.

One of skill in the art may use the crystal structure coordinates, along with the software package Quanta to interactively model the movement of the L11 N terminus as a rigid body relative to the other GAR surfaces. This model will provide information on the many possible interactions between the L11 N terminus and the other amino acid and nucleotide residues comprising the GAR, as well as solvent interactions.

To develop a more detailed picture of the molecular interactions involving the L11 N terminal lobe in the GAR, the software packages CHARMM and AMBER may be applied by one of skill in the art to the crystal structure coordinates. These will provide a molecular

dynamics simulation of the N terminal lobe of L11 within the L11/ GAR RNA complex.

Similarly, CHARMM may be used by one of skill in the art to provide a normal mode dynamics simulation of the L11 N terminal lobe within the L11/GAR context.

Finally, the crystal structure coordinates allow the use of software packages such as DOCK or to simulate docking of the known GAR modulators thiostrepton and micrococcin with the GAR, thereby providing a finely detailed description of those interactions within the GAR critical to its function.

Used in combination, the software approaches described above can manipulate the crystal structure coordinate data to provide a very high resolution three dimensional model of the L11 N terminal lobe and its interactions with other portions of the GAR including van der Waals contacts, electrostatic interactions and hydrogen bonding opportunities.

2. Design of a candidate modulator compound.

Once a detailed three dimensional model of the L11/GAR has been created as described above, one of skill in the art may use the grid-based software approaches GRID or CERIUS II, and MCSS techniques (see, for example, Castro et al., 1999, Medicinal Chem. Res. 9: 98-107) to map favorable interaction positions for functional groups such as protons, hydroxyl groups, anime groups, divalent cations, aromatic and aliphatic functional groups, acetamide, methanol, etc. Once a set of favorable groups for each position are predicted, one of skill in the art may take one of two different approaches to designing a modulator.

First, one may assemble the moieties predicted to interact with the various critical parts of the L11/GAR surfaces into a single molecule. This may be accomplished by one of skill in the art using the software packages CAVEAT, MACCS-3D or HOOK. One of skill in the art may then synthesize the selected compounds for in vitro and in vivo testing for effects on GAR activity.

Alternatively, one may screen a database, such as the MDL Available Chemical Directory to potentially find existing compounds that combine the required moieties in a favorable conformation for GAR binding. The software packages Catalyst, DOCK and FLEXX may be used to advantage for this purpose by one of skill in the art.

EXAMPLE 3. Assaying the Activity of a Candidate Modulator by Displacement of Thiostrepton from the GAR

Thiostrepton binding to GTPase centre RNA can be monitored by a filter binding assays (Uchiumi et al., 1995, Biol. Chem., 270(50):29889-93; Draper et al., 1988, Methods Enzymol., 164:203-20). The filter binding assay can be transformed to a 96-well format using Millipore MHAB (mixed cellulose ester) 96-well plates. The dissociation constant for the thiostrepton/GTPase centre-59mer complex of 1uM is in good accordance with the literature. Additionally, filter binding can show the cooperativity in binding of thiostrepton and L11. Thermotoga maritima ribosomes are known to be sensitive to thiostrepton (Londei et al., 1988, J. Bacteriol., 170(9):4353-60), although 100-fold less than B. stearothermophilus ribosomes. The affinity of thiostrepton for Thermotoga GTPase center RNA in vitro has not yet been determined.

^{35}S- or ^{32}P-labelled RNA is prepared by transcription in the presence of radiolabelled nucleotides. The labelled RNAs are purified by gel electrophoresis or chromatography by reverse-phase. For filter binding assays the RNA are renatured and 3,000 to 10,000 cpm of RNA are used per assay. Association constants between RNA and thiostrepton in the presence or absence of inhbitor are determined in 100 ul reactions containing 10 mM Tris-HCl (pH 7.4), 3 mM MgCl2, 175 mM NH4Cl and 5% v/v DMSO. The reaction mixtures also contain between 2 and 10 uM thiostrepton and a range of inhibitor

concentrations up to 50 uM. The RNA-thiostrepton-inhibitor mixtures are incubated for 15 min at room temperature (approximately 22°C) prior to filtration through the nitrocellulose filter membranes.

For high-throughput screening, the assay can be performed in 96-well filter plates (Multiscreen HA filtration plates, Millipore) with nitrocellulose membranes incorporated into the bottom of each well and filtered using Multiscreen vacuum Manifold (Millipore). The filters

are washed once with 100 ul buffer before determining their radioactivities using Microbeta Liquid Scintillation Counter (Wallac).

The relative amounts of RNA retained in the presence and absence of inhibitor can be determined by quantitation of the radioactivity on each filter. Compounds that reduce the amount of RNA retained on the filter in a concentration dependent manner are competitive inhibitors of thiostrepton binding to the RNA.

EXAMPLE 4. Binding assays with radioactive thiostrepton

Binding of [^{35}S]-labelled thiostrepton to 23S RNA and ribosomes has been shown by gel filtration of RNA and RNA/L11 complexes together with thiostrepton as well as by charcoal (Norit) absorption of unbound [^{35}S]thiostrepton (Thompson et al., 1979. Eur. J. Biochem., 98(1):261-5). Using equilibrium dialysis, the dissociation constant of thiostrepton/23S RNA has been determined as 0.23uM (Thompson & Cundliffe, 1991, Biochimie 1991, 73(7-8):1131-5). The affinity to intact ribosomes is 100-1000fold higher (Pestka et al., 1976, Anal. Biochem., 71(1):137-42).

The ability of biotinylated GTPase centre-59mer to bind thiostrepton (as shown by filter binding) gives a route for a displacement assay employing displacement of

[^{3}H]-labelled thiostrepton (Amersham) from an immobilised GTPase centre RNA/L11 complex or from ribosomes.

EXAMPLE 5. Luciferase translation assay

Using an E. coli S30 lysate and luciferase mRNA (Promega E. coli S30 extract system for linear templates; Cat No: L1030) the active luciferase protein can be synthesised in vitro and the relative amount of luciferase generated is monitored in a bioluminescence assay. The mRNA is either provided by coupled transcription/translation using the linearized plasmid pBESTLucTM as a template or by adding purified luciferase mRNA.

The addition of ribosome-inactivating compounds or antibiotics directed to protein biosynthesis (thiostrepton, kanamycin, chloramphenicol and others) leads to a decrease in yield of active luciferase compared to the control. Compound and antibiotic titrations can be used to determine IC50 values (see Langer et al., 1996, Anal. Biochem., 243(1):150-3).

EXAMPLE 6. Additional translation assays

An S30 transcription/translation system (Promega) can be used to incorporate [^{35}S]methionine into protein translated from MS2 phage RNA. Translation yield is quantified after alkaline hydrolysis by acid precipitation of the synthesised peptides and scintillation counting. Whole-cell protein synthesis can be measured adding [^{14}C]leucine to exponentially growing E. coli cells and measuring the incorporation into protein by alkaline hydrolysis and TCA precipitation (see Shinabarger et al., 1997, Antimicrob. Agents Chemother., 41(10):2132-6).

EXAMPLE 7. Assay of Translation Elongation

Translation elongation is measured using isolated polysomes from E. coli MRE600 (Girbes et al., 1979, Methods Enzymol., 59:353-62), S100 extract from E. coli and poly(U) (Sigma) as a template (e.g. Grise-Miron et al., 1981, Biochim. Biophys. Acta, 656(1):103-10). Incorporation of [^{3}H]phenylalanine into polyphenylalanine is quantified by acid precipitation and

scintillation counting.

EXAMPLE 8. In vitro EF-G-dependent GTP Hydrolysis

Thiostrepton acts on the tRNA translocation step of translation elongation and inhibits elongation factor G (EF-G)-dependent GTP hydrolysis (Pestka et al., 1970, Biochem. Biophys. Res. Commun., 40(3):667-74; Rodnina et al., 1997, Nature, 385:37-41). EF-G is known to contact the GTPase centre region of 23S RNA (Skold et al., 1983, Nucleic Acids Res., 11(14):4923-32; Moazed & Noller, 1986, Nature, 334:362-4). 70S ribosomes support GTP hydrolysis by EF-G in the absence of other factors normally necessary for protein synthesis. Uncoupled GTP hydrolysis and the inhibition by thiostrepton or other compounds can be measured in an assay containing purified ribosomes, purified EF-G and gamma-[^{32}P]-GTP (Stark&Cundliffe, 1979, J. Mol. Biol., 134(4):767-9; Lill et al., 1988, EMBO J., 8(12):3933-8).

References

Abrahams, J. P., and Leslie, A. G. W. (1996). Methods used in the structure determination of bovine mitochondrial F1 ATPase. Acta Cryst. *D52*, 30-42.

Briones, E., Briones, C., Remacha, M., and Ballesta, J. P. (1998). The GTPase center protein L12 is required for correct ribosomal stalk assembly but not for Saccharomyces cerevisiae viability. J Biol Chem *273*, 31956-61.

Brünger, A. T. (1988). Crystallographic refinement by simulated annealing. Application to a 2.8 Å structure of aspartate aminotransferase. J. Mol. Biol. *203*, 803-16.

Bukhman, Y. V., and Draper, D. E. (1997). Affinities and selectivities of divalent cation binding sites within an RNA tertiary structure. J Mol Biol *273*, 1020-31.

Carson, M. (1991). Ribbons 2.0. J.Appl.Cryst. *24*, 958-961.

Cate, J., Gooding, A., Podell, E., Zhou, K., Golden, B., Szewczack, A., Kundrot, C., Cech, T., and Doudna, J. (1996). RNA Tertiary Structure Mediation by Adenosine Platforms. Science *273*, 1696-1699.

Cate, J. H., Gooding, A. R., Podell, E., Zhou, K., Golden, B. L., Kundrot, C. E., Cech, T. R., and Doudna, J. A. (1996). Crystal structure of a group I ribozyme domain: principles of RNA packing. Science *273*, 1678-85.

Conn, G. L., Gutell, R. R., and Draper, D. E. (1998). A functional ribosomal RNA tertiary structure involves a base triple interaction. Biochemistry *37*, 11980-8.

Cundliffe, E. (1986). Involvement of specific portions of rRNA in defined ribosomal functions: a study utilizing antibiotics. In Structure, Function and Genetics of Ribosomes, B. Hardesty and G. Kramer, eds. (New York: Springer-Verlag), pp. 586-604.

Cundliffe, E., and Thompson, J. (1981). Concerning the mode of action of micrococcin upon bacterial protein synthesis. Eur J Biochem *118*, 47-52.

Cundliffe, E., and Thompson, J. (1979). Ribose methylation and resistance to thiostrepton. Nature *278*, 859-61.

de la Fortelle, E., and Bricogne, G. (1997). Maximum-likelihood heavy-atom parameter refinement for multiple isomorphous replacement and multiwavelength anomalous diffraction methods. In Methods in Enzymology, C. W. Carter, Jr. and R. M. Sweet, eds. (New York: Academic Press), pp. 472-93.

Donner, D., Villems, R., Liljas, A., and Kurland, C. G. (1978). Guanosinetriphosphatase activity dependent on elongation factor Tu and ribosomal protein L7/L12. Proc Natl Acad Sci U S A *75*, 3192-5.

Draper, D. E., and Xing, Y. (1995). Protein recognition of a ribosomal RNA tertiary structure. Nucleic Acids Symp Ser *33*, 5-7.

Engh, R. A., and Huber, R. (1991). Accurate bond and angle parameters for x-ray protein

structure refinement. Acta Cryst. *A47*, 392-400.

Ferre-D'Amare, A. R., Zhou, K., and Doudna, J. A. (1998). Crystal structure of a hepatitis delta virus ribozyme. Nature *395*, 567-74.

Fountain, M. A., Serra, M. J., Krugh, T. R., and Turner, D. H. (1996). Structural features of a six-nucleotide RNA hairpin loop found in ribosomal RNA. Biochemistry *35*, 6539-48.

Glotz, C., Zwieb, C., Brimacombe, R., Edwards, K., and Kössel, H. (1981). Secondary structure of the large subunit ribosomal RNA from Escherichia coli, Zea mays chloroplast, and human and mouse mitochondrial ribosomes. Nucleic Acids Res *9*, 3287-306.

Gruenwedel, D. W., and Davidson, N. (1966). Complexing and denaturation of DNA by methylmercuric hydroxide. I. Spectrophotometric studies. J Mol Biol *21*, 129-44.

Gruenwedel, D. W., and Davidson, N. (1967). Complexing and denaturation of DNA by methylmercuric hydroxide. II. Ultracentrifugation studies. Biopolymers *5*, 847-61.

Hendrickson, W. A. (1991). Determination of macromolecular structures from anomalous diffraction of synchrotron radiation. Science *254*, 51-58.

Hinck, A. P., Markus, M. A., Huang, S., Grzesiek, S., Kustonovich, I., Draper, D. E., and Torchia, D. A. (1997). The RNA binding domain of ribosomal protein L11: three-

dimensional structure of the RNA-bound form of the protein and its interaction with 23 S rRNA. J Mol Biol *274*, 101-13.

Jones, T. A., and Kjeldgaard, M. (1997). Electron-density map interpretation. Meth. Enzymol. *277B*, 173-207.

Kosturko, L. D., Folzer, C., and Stewart, R. F. (1974). The crystal and molecular structure of a 2:1 complex of 1-methylthymine- mercury (II). Biochemistry *13*, 3949-52.

Kraulis, P. (1991). MOLSCRIPT: A program to produce both detailed and schematic plots of protein structures. J. Appl. Crystallogr. *24*, 946-50.

Lu, M., and Draper, D. E. (1994). Bases defining an ammonium and magnesium ion-dependent tertiary structure within the large subunit ribosomal RNA. J Mol Biol *244*, 572-85.

Lu, M., and Draper, D. E. (1995). On the role of rRNA tertiary structure in recognition of ribosomal protein L11 and thiostrepton. Nucleic Acids Res *23*, 3426-33.

Markus, M. A., Hinck, A. P., Huang, S., Draper, D. E., and Torchia, D. A. (1997). High resolution solution structure of ribosomal protein L11-C76, a helical protein with a flexible loop that becomes structured upon binding to RNA. Nat Struct Biol *4*, 70-7.

Moazed, D., Robertson, J. M., and Noller, H. F. (1988). Interaction of elongation factors EF-

G and EF-Tu with a conserved loop in 23S RNA. Nature *334*, 362-4.

Munishkin, A., and Wool, I. G. (1997). The ribosome-in-pieces: binding of elongation factor EF-G to oligoribonucleotides that mimic the sarcin/ricin and thiostrepton domains of 23S ribosomal RNA. Proc Natl Acad Sci U S A *94*, 12280-4.

Nicholls, A., Sharp, K. A., and Honig, B. (1991). Protein folding and association: insights from the interfacial and thermodynamic properties of hydrocarbons. Proteins *11*, 281-96.

Nissen, P., Kjeldgaard, M., Thirup, S., Polekhina, G., Reshetnikova, L., Clark, B. F., and Nyborg, J. (1995). Crystal structure of the ternary complex of Phe-tRNAPhe, EF-Tu, and a GTP analog. Science *270*, 1464-72.

Noller, H. F., Kop, J., Wheaton, V., Brosius, J., Gutell, R. R., Kopylov, A. M., Dohme, F., Herr, W., Stahl, D. A., Gupta, R., and Waese, C. R. (1981). Secondary structure model for 23S ribosomal RNA. Nucleic Acids Res *9*, 6167-89.

Otwinowski, Z., and Minor, W. (1997). Processing of x-ray diffraction data collected in oscillation mode. In Methods in Enzymology, C. W. J. Carter and R. M. Sweet, eds. (New York: Academic Press), pp. 307-25.

Parkinson, G., Vojtechovsky, J., Clowney, L., Brünger, A. T., and Berman, H. M. (1996). New parameters for the refinement of nucleic acid containing structures. Acta Cryst. *D52*, 57-

64.

Pestka, S. (1970). Thiostrepton: a ribosomal inhibitor of translocation. Biochem Biophys Res Commun *40*, 667-74.

Porse, B. T., Cundliffe, E., and Garrett, R. A. (1999). The antibiotic micrococcin acts on protein L11 at the ribosomal GTPase centre. J. Mol. Biol. *287*, 33-45.

Porse, B. T., Leviev, I., Mankin, A. S., and Garrett, R. A. (1998). The antibiotic thiostrepton inhibits a functional transition within protein L11 at the ribosomal GTPase centre. J Mol Biol *276*, 391-404.

Price, S. R., Ito, N., Oubridge, C., Avis, J. M., and Nagai, K. (1995). Crystallisation of RNA-protein complexes. I. Methods for the large-scale preparation of RNA suitable for crystallographic studies. J. Mol. Biol. *249*, 398-408.

Quigley, G. J., and Rich, A. (1976). Structural domains of transfer RNA molecules. Science *194*, 796-806.

Ramakrishnan, V., and Biou, V. (1997). Treatment of multiwavelength anomalous diffraction data as a special case of multiple isomorphous replacement. In Meth. Enzymol., C. W. Carter, Jr. and R. M. Sweet, eds. (New York: Academic Press), pp. 538-57.

Ramakrishnan, V., Finch, J. T., Graziano, V., Lee, P. L., and Sweet, R. M. (1993). Crystal structure of globular domain of histone H5 and its implications for nucleosome binding. Nature *362*, 219-23.

Ramakrishnan, V., and White, S. W. (1998). Ribosomal protein structures: insights into the architecture, machinery and evolution of the ribosome. Trends Biochem Sci *23*, 208-12.

Rodnina, M. V., Savelsbergh, A., Katunin, V. I., and Wintermeyer, W. (1997). Hydrolysis of GTP by elongation factor G drives tRNA movement on the ribosome. Nature *385*, 37-41.

Rosendahl, G., and Douthwaite, S. (1994). The antibiotics micrococcin and thiostrepton interact directly with 23S rRNA nucleotides 1067A and 1095A. Nucleic Acids Res *22*, 357-63.

Rosendahl, G., and Douthwaite, S. (1993). Ribosomal proteins L11 and L10.(L12)4 and the antibiotic thiostrepton interact with overlapping regions of the 23 S rRNA backbone in the ribosomal GTPase centre. J Mol Biol *234*, 1013-20.

Schmidt, F. J., Thompson, J., Lee, K., Dijk, J., and Cundliffe, E. (1981). The binding site for ribosomal protein L11 within 23 S ribosomal RNA of Escherichia coli. J Biol Chem *256*, 12301-5.

Sopori, M. L., and Lengyel, P. (1972). Components of the 50S ribosomal subunit involved in

GTP cleavage. Biochem Biophys Res Commun *46*, 238-44.

Spahn, C. M., and Nierhaus, K. H. (1998). Models of the elongation cycle: an evaluation. Biol Chem *379*, 753-72.

Stöffler, G., Cundliffe, E., Stoffler-Meilicke, M., and Dabbs, E. R. (1980). Mutants of Escherichia coli lacking ribosomal protein L11. J Biol Chem *255*, 10517-22.

Studier, F. W., Rosenberg, A. H., Dunn, J. J., and Dubendorff, J. W. (1990). Use of T7 RNA polymerase to direct expression of cloned genes. Meth. Enzymol. *185*, 61-89.

Szewczak, A. A., Moore, P. B., Chang, Y. L., and Wool, I. G. (1993). The conformation of the sarcin/ricin loop from 28S ribosomal RNA. Proc Natl Acad Sci U S A *90*, 9581-5.

Terwilliger, T., and Berendzen, J. (1999). Automated MAD and MIR structure determination. Acta Cryst *D (in press)*.

Thompson, J., Cundliffe, E., and Stark, M. (1979). Binding of thiostrepton to a complex of 23-S rRNA with ribosomal protein L11. Eur J Biochem *98*, 261-5.

Thompson, J., Schmidt, F., and Cundliffe, E. (1982). Site of action of a ribosomal RNA methylase conferring resistance to thiostrepton. J Biol Chem *257*, 7915-7.

Wang, Y. X., Lu, M., and Draper, D. E. (1993). Specific ammonium ion requirement for functional ribosomal RNA tertiary structure. Biochemistry *32*, 12279-82.

Wilson, K. S., and Noller, H. F. (1998). Mapping the position of translational elongation factor EF-G in the ribosome by directed hydroxyl radical probing. Cell *92*, 131-9.

Wilson, K. S., and Noller, H. F. (1998). Molecular movement inside the translational engine. Cell *92*, 337-49.

Wimberly, B. (1994). A common RNA loop motif as a docking module and its function in the hammerhead ribozyme. Nat Struct Biol *1*, 820-7.

Wimberly, B., Varani, G., and Tinoco, I., Jr. (1993). The conformation of loop E of eukaryotic 5S ribosomal RNA. Biochemistry *32*, 1078-87.

Wimberly, B. T., White, S. W., and Ramakrishnan, V. (1997). The structure of ribosomal protein S7 at 1.9 A resolution reveals a beta-hairpin motif that binds double-stranded nucleic acids. Structure *5*, 1187-98.

Xing, Y., and Draper, D. E. (1996). Cooperative interactions of RNA and thiostrepton antibiotic with two domains of ribosomal protein L11. Biochemistry *35*, 1581-8.

Xing, Y., and Draper, D. E. (1995). Stabilization of a ribosomal RNA tertiary structure by

ribosomal protein L11. J Mol Biol *249*, 319-31.

Xing, Y., Guha Thakurta, D., and Draper, D. E. (1997). The RNA binding domain of ribosomal protein L11 is structurally similar to homeodomains. Nat Struct Biol *4*, 24-7.

Table I
Crystallographic statistics

Data collection

	λ1 (1.008 Å)	λ2 (0.980 Å)
Reflections	104,096	107,907
Independent reflections	25,927	25,894
Completeness	99% (98%)*	98% (97%)*
Mean (I / sigma (I))	20 (4.2)*	20 (4.5)*
R_{sym}	4.1% (17%)*	4.2% (17%)*
d_{min} (Å)	2.6	2.6
f' (Hg) (electrons)**	-12.0	-9.0
f'' (Hg) (electrons)**	6.4	8.0
f' (Cd) (electrons)**	-0.42	-0.46
f'' (Cd) (electrons)**	2.3	2.2

*Values in parentheses refer to the highest resolution shell.
**Values after SHARP refinement.

Phasing

	λ1-λ2 isomorphous anomalous	λ1 anomalous	λ2
R_{Cullis} (centrics)	0.50	--	--
R_{Kraut} (acentrics)	0.09	0.025	0.023
Phasing power (acentrics)	1.25	1.54	1.52

Mean figure of merit (acentrics) 0.39
Mean figure of merit (centrics) 0.23

Refinement

Number of atoms	4196 (2474 RNA, 1524 protein, 198 water & ions)
R_{cryst} / R_{free} (5% of data)	0.228 / 0.253

RMS deviation from ideal geometry

bond lengths	0.005 Å
bond angles	1.2 degrees

TABLE II

```
HEADER    RNA-PROTEIN COMPLEX                    14-APR-99
ONHOLD    ONE-YEAR HOLD; EXPERIMENTAL DATA, ONE-YEAR HOLD
TITLE     CRYSTAL STRUCTURE OF THE RIBOSOMAL PROTEIN L11-RNA COMPLEX

COMPND    MOL_ID: 1;
COMPND   2 MOLECULE: 23S RIBOSOMAL RNA;
COMPND   3 CHAIN: C, D;
COMPND   4 FRAGMENT: FRAGMENT 1051-1108;
COMPND   5 MUTATION: U1108C;
COMPND   6 OTHER_DETAILS: COVALENT MERCURY LIGAND AT U1061;
COMPND   7 MOL_ID: 2;
COMPND   8 MOLECULE: RIBOSOMAL PROTEIN L11;
COMPND   9 CHAIN: A, B;
COMPND  10 ENGINEERED: YES;
COMPND  11 OTHER_DETAILS: COVALENT MERCURY LIGAND AT CYS39

SOURCE    MOL_ID: 1;
SOURCE   2 ORGANISM_SCIENTIFIC: THERMOTOGA MARITIMA;
SOURCE   3 OTHER_DETAILS: IN VITRO TRANSCRIBED RNA;
SOURCE   4 MOL_ID: 2;
SOURCE   5 ORGANISM_SCIENTIFIC: THERMOTOGA MARITIMA;
SOURCE   6 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
SOURCE   7 EXPRESSION_SYSTEM_STRAIN: BL21(DE3);
SOURCE   8 EXPRESSION_SYSTEM_PLASMID: PET13A;
SOURCE   9 OTHER_DETAILS: RECOMBINANT PROTEIN
KEYWDS    RNA-PROTEIN COMPLEX, RNA, RIBOSOME, TRANSLOCATION,

KEYWDS   2 THIOSTREPTON
EXPDTA    X-RAY DIFFRACTION
AUTHOR    B.T.WIMBERLY,R.GUYMON,J.P.MCCUTCHEON,S.W.WHITE,
AUTHOR   2 V.RAMAKRISHNAN
REMARK    1
REMARK    1 REFERENCE 1
REMARK    1  AUTH   Y.XING,D.DRAPER
REMARK    1  TITL   COOPERATIVE INTERACTIONS OF RNA AND THIOSTREPTON

REMARK    1  TITL 2 ANTIBIOTIC WITH TWO DOMAINS OF RIBOSOMAL PROTEIN

REMARK    1  TITL 3 L11
REMARK    1  REF    BIOCHEMISTRY                V. 35  1581 1996
REMARK    1  REFN   ASTM BICHAW  US ISSN 0006-2960            0033
REMARK    1 REFERENCE 2
REMARK    1  AUTH   J.THOMPSON,F.SCHMIDT,E.CUNDLIFFE
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REMARK  1 TITL   SITE OF ACTION OF A RIBOSOMAL RNA METHYLASE
REMARK  1 TITL 2 CONFERRING RESISTANCE TO THIOSTREPTON
REMARK  1 REF    J.BIOL.CHEM.              V. 257  7915 1982
REMARK  1 REFN   ASTM JBCHA3  US ISSN 0021-9258           0071
REMARK  1 REFERENCE 3
REMARK  1 AUTH   J.THOMPSON,E.CUNDLIFFE,M.STARK
REMARK  1 TITL   BINDING OF THIOSTREPTON TO A COMPLEX OF 23S RNA
REMARK  1 TITL 2 WITH RIBOSOMAL PROTEIN L11
REMARK  1 REF    EUR.J.BIOCHEM.            V. 98   261 1979
REMARK  1 REFN   ASTM EJBCAI  IX ISSN 0014-2956           0262
REMARK  2
REMARK  2 RESOLUTION. 2.57 ANGSTROMS.
REMARK  3
REMARK  3 REFINEMENT.
REMARK  3  PROGRAM     : X-PLOR 3.851
REMARK  3  AUTHORS     : BRUNGER
REMARK  3
REMARK  3  DATA USED IN REFINEMENT.
REMARK  3  RESOLUTION RANGE HIGH (ANGSTROMS) : 2.57
REMARK  3  RESOLUTION RANGE LOW  (ANGSTROMS) : 20.0
REMARK  3  DATA CUTOFF          (SIGMA(F)) : 0.0
REMARK  3  DATA CUTOFF HIGH         (ABS(F)) : 1000000.0
REMARK  3  DATA CUTOFF LOW          (ABS(F)) : 0.001
REMARK  3  COMPLETENESS (WORKING+TEST)   (%) : 95.5
REMARK  3  NUMBER OF REFLECTIONS             : 49313
REMARK  3
REMARK  3  FIT TO DATA USED IN REFINEMENT.
REMARK  3  CROSS-VALIDATION METHOD       : THROUGHOUT
REMARK  3  FREE R VALUE TEST SET SELECTION  : RANDOM
REMARK  3  R VALUE            (WORKING SET) : 0.219
REMARK  3  FREE R VALUE                     : 0.254
REMARK  3  FREE R VALUE TEST SET SIZE   (%) : 4.9
REMARK  3  FREE R VALUE TEST SET COUNT      : 2398
REMARK  3  ESTIMATED ERROR OF FREE R VALUE  : 0.005
REMARK  3
REMARK  3  FIT IN THE HIGHEST RESOLUTION BIN.
REMARK  3  TOTAL NUMBER OF BINS USED         : 6
REMARK  3  BIN RESOLUTION RANGE HIGH      (A) : 2.57
REMARK  3  BIN RESOLUTION RANGE LOW       (A) : 2.73
REMARK  3  BIN COMPLETENESS (WORKING+TEST) (%) : 86.2
REMARK  3  REFLECTIONS IN BIN    (WORKING SET) : 7101
REMARK  3  BIN R VALUE           (WORKING SET) : 0.386
REMARK  3  BIN FREE R VALUE                    : 0.432
REMARK  3  BIN FREE R VALUE TEST SET SIZE  (%) : 4.5
REMARK  3  BIN FREE R VALUE TEST SET COUNT     : 331
```

REMARK 3 ESTIMATED ERROR OF BIN FREE R VALUE : 0.024
REMARK 3
REMARK 3 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.

REMARK 3 PROTEIN ATOMS : 1524
REMARK 3 NUCLEIC ACID ATOMS : 2474
REMARK 3 HETEROGEN ATOMS : 35
REMARK 3 SOLVENT ATOMS : 142
REMARK 3
REMARK 3 B VALUES.
REMARK 3 FROM WILSON PLOT (A**2) : 58.8
REMARK 3 MEAN B VALUE (OVERALL, A**2) : 42.8
REMARK 3 OVERALL ANISOTROPIC B VALUE.
REMARK 3 B11 (A**2) : NULL
REMARK 3 B22 (A**2) : NULL
REMARK 3 B33 (A**2) : NULL
REMARK 3 B12 (A**2) : NULL
REMARK 3 B13 (A**2) : NULL
REMARK 3 B23 (A**2) : NULL
REMARK 3
REMARK 3 ESTIMATED COORDINATE ERROR.
REMARK 3 ESD FROM LUZZATI PLOT (A) : 0.32
REMARK 3 ESD FROM SIGMAA (A) : 0.45
REMARK 3 LOW RESOLUTION CUTOFF (A) : 5.00
REMARK 3
REMARK 3 CROSS-VALIDATED ESTIMATED COORDINATE ERROR.
REMARK 3 ESD FROM C-V LUZZATI PLOT (A) : 0.39
REMARK 3 ESD FROM C-V SIGMAA (A) : 0.50
REMARK 3
REMARK 3 RMS DEVIATIONS FROM IDEAL VALUES.
REMARK 3 BOND LENGTHS (A) : 0.005
REMARK 3 BOND ANGLES (DEGREES) : 1.0
REMARK 3 DIHEDRAL ANGLES (DEGREES) : 28.8
REMARK 3 IMPROPER ANGLES (DEGREES) : 1.40
REMARK 3
REMARK 3 ISOTROPIC THERMAL MODEL : RESTRAINED
REMARK 3
REMARK 3 ISOTROPIC THERMAL FACTOR RESTRAINTS. RMS SIGMA
REMARK 3 MAIN-CHAIN BOND (A**2) : 3.59 ; 1.50
REMARK 3 MAIN-CHAIN ANGLE (A**2) : 5.28 ; 2.00
REMARK 3 SIDE-CHAIN BOND (A**2) : 6.59 ; 2.00
REMARK 3 SIDE-CHAIN ANGLE (A**2) : 9.24 ; 2.50
REMARK 3
REMARK 3 NCS MODEL : RESTRAINTS
REMARK 3

```
REMARK   3 NCS RESTRAINTS.                      RMS   SIGMA/WEIGHT
REMARK   3  GROUP  1 POSITIONAL         (A) : 0.07  ; 50
REMARK   3  GROUP  1 B-FACTOR          (A**2) : 5.51  ; 2
REMARK   3  GROUP  2 POSITIONAL         (A) : 0.07  ; 50
REMARK   3  GROUP  2 B-FACTOR          (A**2) : 5.51  ; 2
REMARK   3
REMARK   3 PARAMETER FILE  1  : DNA-RNA-MULTI-ENDO.PARAM
REMARK   3 PARAMETER FILE  2  : PROTEIN_REP.PARAM
REMARK   3 TOPOLOGY FILE  1   : DNA-RNA-MULTI-ENDO.TOP
REMARK   3 TOPOLOGY FILE  2   : TOPHCSDX.PRO
REMARK   3 TOPOLOGY FILE  3   : TOPH19.SOL
REMARK   3
REMARK   3 OTHER REFINEMENT REMARKS: NCS RESTRAINTS APPLIED TO RNA

REMARK   3 THROUGHOUT, NOT TO PROTEIN
REMARK   5
REMARK   5 WARNING
REMARK   5    : THIS IS LAYER 1 RELEASE.
REMARK   5
REMARK   5 PLEASE NOTE THAT THIS ENTRY WAS RELEASED AFTER DEPOSITOR
REMARK   5 CHECKING AND APPROVAL BUT WITHOUT PDB STAFF
INTERVENTION.
REMARK   5 AN AUXILIARY FILE, AUX    .RPT, IS AVAILABLE FROM THE
REMARK   5 PDB FTP SERVER AND IS ACCESSIBLE THROUGH THE 3DB BROWSER.
REMARK   5 THE FILE CONTAINS THE OUTPUT OF THE PROGRAM WHAT_CHECK
AND
REMARK   5 OTHER DIAGNOSTICS.
REMARK   5
REMARK   5 NOMENCLATURE IN THIS ENTRY, INCLUDING HET RESIDUE NAMES
REMARK   5 AND HET ATOM NAMES, HAS NOT BEEN STANDARDIZED BY THE PDB
REMARK   5 PROCESSING STAFF.  A LAYER 2 ENTRY WILL BE RELEASED SHORTLY
REMARK   5 AFTER THIS STANDARDIZATION IS COMPLETED AND APPROVED BY
THE
REMARK   5 DEPOSITOR.  THE LAYER 2 ENTRY WILL BE TREATED AS A
REMARK   5 CORRECTION TO THIS ONE, WITH THE APPROPRIATE REVDAT
RECORD.
REMARK   5
REMARK   5 FURTHER INFORMATION INCLUDING VALIDATION CRITERIA USED IN
REMARK   5 CHECKING THIS ENTRY AND A LIST OF MANDATORY DATA FIELDS
REMARK   5 ARE AVAILABLE FROM THE PDB WEB SITE AT
REMARK   5 HTTP://WWW.PDB.BNL.GOV/.
REMARK   6
REMARK   6 THE ASYMMETRIC UNIT CONTAINS TWO L11-RNA COMPLEXES.
COMPLEX
REMARK   6 1 CONSISTS OF CHAINS A AND C, AND COMPLEX 2 CONSISTS OF
```

REMARK 6 CHAINS B AAND D. RESIDUES 1-7 AND 141 OF CHAIN A ARE
REMARK 6 DISORDERED. THE DENSITY FOR RESIDUES 8-70 OF CHAIN A WAS OF

REMARK 6 SIGNIFICANTLY LOWER QUALITY THAN THE DENSITY FOR THE

REMARK 6 REMAINDER OF THE ASYMMETRIC UNIT, AND THE QUALITY OF THE

REMARK 6 MODEL FOR THIS N-TERMINAL DOMAIN IS LOWER THAN THAT OF
THE
REMARK 6 C-TERMINAL DOMAIN (RESIDUES 71-140). RESIDUES 1-70 AND 141
REMARK 6 OF CHAIN B ARE DISORDERED. THE RNA IS NUMBERED WITH THE E.

REMARK 6 COLI NUMBERING TO FACILITATE COMPARISON WITH THE
EXTENSIVE
REMARK 6 BIOCHEMICAL DATA ON THE E. COLI RNA-L11 SYSTEM. THE E. COLI

REMARK 6 RNA NUMBERING IS ALSO USED IN THE PRIMARY REFERENCE

REMARK 6 DESCRIBING THIS STRUCTURE.
REMARK 7
REMARK 7 TER
REMARK 7 ASP: TERMINAL RESIDUE NOT SEEN IN MAPS
REMARK 7 ASP: TERMINAL RESIDUE NOT SEEN IN MAPS
REMARK 200
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200 EXPERIMENT TYPE : X-RAY DIFFRACTION
REMARK 200 DATE OF DATA COLLECTION : 24-SEP-1998
REMARK 200 TEMPERATURE (KELVIN) : 100
REMARK 200 PH : 8.3
REMARK 200 NUMBER OF CRYSTALS USED : 1
REMARK 200
REMARK 200 SYNCHROTRON (Y/N) : Y
REMARK 200 RADIATION SOURCE : NSLS
REMARK 200 BEAMLINE : X12C
REMARK 200 X-RAY GENERATOR MODEL : NULL
REMARK 200 MONOCHROMATIC OR LAUE (M/L) : M
REMARK 200 WAVELENGTH OR RANGE (A) : 0.98,1.01
REMARK 200 MONOCHROMATOR : SI CRYSTAL
REMARK 200 OPTICS : MIRRORS
REMARK 200
REMARK 200 DETECTOR TYPE : BRANDEIS 1K X 1 K CCD
REMARK 200 DETECTOR MANUFACTURER : NULL
REMARK 200 INTENSITY-INTEGRATION SOFTWARE : DENZO
REMARK 200 DATA SCALING SOFTWARE : SCALEPACK

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REMARK 200
REMARK 200  NUMBER OF UNIQUE REFLECTIONS   : 49313
REMARK 200  RESOLUTION RANGE HIGH      (A) : 2.57
REMARK 200  RESOLUTION RANGE LOW       (A) : 20.0
REMARK 200  REJECTION CRITERIA  (SIGMA(I)) : 0
REMARK 200
REMARK 200 OVERALL.
REMARK 200  COMPLETENESS FOR RANGE     (%) : 95.5
REMARK 200  DATA REDUNDANCY                : 4.0
REMARK 200  R MERGE                    (I) : NULL
REMARK 200  R SYM                      (I) : 0.041
REMARK 200  &LT;I/SIGMA(I)&GT; FOR THE DATA SET  : 20
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 2.57
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE LOW  (A) : 2.73
REMARK 200  COMPLETENESS FOR SHELL     (%) : 86.2
REMARK 200  DATA REDUNDANCY IN SHELL       : 3.4
REMARK 200  R MERGE FOR SHELL          (I) : NULL
REMARK 200  R SYM FOR SHELL            (I) : 0.17
REMARK 200  &LT;I/SIGMA(I)&GT; FOR SHELL       : 4.3
REMARK 200
REMARK 200 DIFFRACTION PROTOCOL: MAD
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: MAD
REMARK 200 SOFTWARE USED: NULL
REMARK 200 STARTING MODEL: NULL
REMARK 200
REMARK 200 REMARK: TWO WAVELENGTH HG MAD
REMARK 280
REMARK 280 CRYSTAL
REMARK 280 SOLVENT CONTENT, VS  (%): 55
REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): 3.1
REMARK 280
REMARK 280 CRYSTALLIZATION CONDITIONS:
REMARK 280 25% GLYCEROL, 15% PEG 4000, 50 MM TRIS PH 7.5,
REMARK 280 50 MM MGCL2, 20 MM CDCL2, 0.2 M KCL,
REMARK 280 1 MM DITHIOTHREITOL, 4 DEGREES C
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 21 21 21
REMARK 290
REMARK 290     SYMOP   SYMMETRY
REMARK 290    NNNMMM   OPERATOR
REMARK 290      1555   X,Y,Z
REMARK 290      2555   1/2-X,-Y,1/2+Z
```

REMARK 290 3555 -X,1/2+Y,1/2-Z
REMARK 290 4555 1/2+X,1/2-Y,-Z
REMARK 290
REMARK 290 WHERE NNN -> OPERATOR NUMBER
REMARK 290 MMM -> TRANSLATION VECTOR
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS

REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM
REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY

REMARK 290 RELATED MOLECULES.
REMARK 290 SMTRY1 1 1.000000 0.000000 0.000000 0.00000
REMARK 290 SMTRY2 1 0.000000 1.000000 0.000000 0.00000
REMARK 290 SMTRY3 1 0.000000 0.000000 1.000000 0.00000
REMARK 290 SMTRY1 2 -1.000000 0.000000 0.000000 31.94480
REMARK 290 SMTRY2 2 0.000000 -1.000000 0.000000 0.00000
REMARK 290 SMTRY3 2 0.000000 0.000000 1.000000 77.76050
REMARK 290 SMTRY1 3 -1.000000 0.000000 0.000000 0.00000
REMARK 290 SMTRY2 3 0.000000 1.000000 0.000000 42.13010
REMARK 290 SMTRY3 3 0.000000 0.000000 -1.000000 77.76050
REMARK 290 SMTRY1 4 1.000000 0.000000 0.000000 31.94480
REMARK 290 SMTRY2 4 0.000000 -1.000000 0.000000 42.13010
REMARK 290 SMTRY3 4 0.000000 0.000000 -1.000000 0.00000
REMARK 290
REMARK 290 REMARK: NULL
REMARK 295
REMARK 295 NON-CRYSTALLOGRAPHIC SYMMETRY
REMARK 295 THE TRANSFORMATIONS PRESENTED ON THE MTRIX RECORDS BELOW
REMARK 295 DESCRIBE NON-CRYSTALLOGRAPHIC RELATIONSHIPS AMONG ATOMS
REMARK 295 IN THIS ENTRY. APPLYING THE APPROPRIATE MTRIX
REMARK 295 TRANSFORMATION TO THE RESIDUES LISTED FIRST WILL YIELD

REMARK 295 APPROXIMATE COORDINATES FOR THE RESIDUES LISTED SECOND.

REMARK 295 CHAIN IDENTIFIERS GIVEN AS "?" REFER TO CHAINS FOR WHICH

REMARK 295 ATOMS ARE NOT FOUND IN THIS ENTRY.
REMARK 295
REMARK 295 APPLIED TO TRANSFORMED TO
REMARK 295 TRANSFORM CHAIN RESIDUES CHAIN RESIDUES RMSD
REMARK 295 SSS

```
REMARK 295   M 1     C 1051 ..1108      D 1051 ..1108     0.07
REMARK 295   M 2     A  71 .. 140       B  71 .. 140      0.99
REMARK 295
REMARK 295   WHERE SSS -&GT; COLUMNS 8-10 OF MTRIX RECORDS
REMARK 295
REMARK 295 REMARK:
REMARK 295 NCS RESTRAINTS NOT APPLIED TO PROTEIN
REMARK 465
REMARK 465 MISSING RESIDUES
REMARK 465 THE FOLLOWING RESIDUES WERE NOT LOCATED IN THE
REMARK 465 EXPERIMENT. (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN

REMARK 465 IDENTIFIER; SSSEQ=SEQUENCE NUMBER; I=INSERTION CODE):

REMARK 465
REMARK 465   M RES C SSSEQI
REMARK 465    ALA A    2
REMARK 465    LYS A    3
REMARK 465    LYS A    4
REMARK 465    VAL A    5
REMARK 465    ALA A    6
REMARK 465    ALA A    7
REMARK 465    ASP A  141
REMARK 465    ALA B    2  TO  ILE B   70
REMARK 465    ASP B  141
REMARK 470
REMARK 470 MISSING ATOM
REMARK 470 THE FOLLOWING RESIDUES HAVE MISSING ATOMS (M=MODEL
NUMBER;
REMARK 470 RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE
NUMBER;
REMARK 470 I=INSERTION CODE):
REMARK 470   M RES CSSEQI  ATOMS
REMARK 470      G C1051    P   O1P  O2P
REMARK 470      G D1051    P   O1P  O2P
REMARK 550
REMARK 550 SEGID
REMARK 550  RNA1, RNA2
REMARK 550  L111, L112
REMARK 600
REMARK 600 HETEROGEN
REMARK 600 THERE ARE A TOTAL OF 8 CADMIUM IONS IN THE STRUCTURE

REMARK 600
REMARK 600 THERE ARE A TOTAL OF 19 MAGNESIUM IONS IN THE STRUCTURE
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REMARK 600
REMARK 600 THERE ARE A TOTAL OF 8 METHYLMERCURY
REMARK 600 IONS IN THE STRUCTURE.
REMARK 600 THE METHYL GROUP HAS NOT BEEN MODELLED
REMARK 600 FOR ANY OF THESE IONS.
REMARK 600 TWO OF THE IONS ARE COVALENTLY BOUND
REMARK 600 TO CYS A 39.
REMARK 600 ONE IS COVALENTLY BOUND TO U C 1061.
REMARK 600 ONE IS COVALENTLY BOUND TO U D 1061.
REMARK 600
REMARK 800
REMARK 800 SITE
REMARK 800 SITE_IDENTIFIER: TSR
REMARK 800 SITE_DESCRIPTION:
REMARK 800 PUTATIVE THIOSTREPTON/MICROCOCCIN BINDING SITE
REMARK 800
REMARK 800 SITE_IDENTIFIER: TSR
REMARK 800 SITE_DESCRIPTION:
REMARK 800 PUTATIVE THIOSTREPTON/MICROCOCCIN BINDING SITE
REMARK 800      ....
REMARK 800 SITE_IDENTIFIER: TSR
REMARK 800 SITE_DESCRIPTION:
REMARK 800 PUTATIVE THIOSTREPTON/MICROCOCCIN BINDING SITE
REMARK 800
DBREF    A   8  140 SWS   P29395  RL11_THEMA     1   141
DBREF    B  71  140 SWS   P29395  RL11_THEMA     1   141
DBREF    C 1051 1108 PDB                1051  1108
DBREF    D 1051 1108 PDB                1051  1108
SEQADV    RES C 1108  GI  M67498      1168 ENGINEERED MUTATION
SEQADV    RES D 1108  GI  M67498      1168 ENGINEERED MUTATION
SEQRES  1 A  140  ALA LYS LYS VAL ALA ALA GLN ILE LYS LEU GLN LEU PRO
SEQRES  2 A  140  ALA GLY LYS ALA THR PRO ALA PRO PRO VAL GLY PRO ALA

SEQRES  3 A  140  LEU GLY GLN HIS GLY VAL ASN ILE MET GLU PHE CYS LYS
SEQRES  4 A  140  ARG PHE ASN ALA GLU THR ALA ASP LYS ALA GLY MET ILE

SEQRES  5 A  140  LEU PRO VAL VAL ILE THR VAL TYR GLU ASP LYS SER PHE
SEQRES  6 A  140  THR PHE ILE ILE LYS THR PRO PRO ALA SER PHE LEU LEU
SEQRES  7 A  140  LYS LYS ALA ALA GLY ILE GLU LYS GLY SER SER GLU PRO
SEQRES  8 A  140  LYS ARG LYS ILE VAL GLY LYS VAL THR ARG LYS GLN ILE
SEQRES  9 A  140  GLU GLU ILE ALA LYS THR LYS MET PRO ASP LEU ASN ALA
SEQRES 10 A  140  ASN SER LEU GLU ALA ALA MET LYS ILE ILE GLU GLY THR
SEQRES 11 A  140  ALA LYS SER MET GLY ILE GLU VAL VAL ASP
SEQRES  1 B  140  ALA LYS LYS VAL ALA ALA GLN ILE LYS LEU GLN LEU PRO
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SEQRES 2 B 140 ALA GLY LYS ALA THR PRO ALA PRO PRO VAL GLY PRO ALA

SEQRES 3 B 140 LEU GLY GLN HIS GLY VAL ASN ILE MET GLU PHE CYS LYS
SEQRES 4 B 140 ARG PHE ASN ALA GLU THR ALA ASP LYS ALA GLY MET ILE

SEQRES 5 B 140 LEU PRO VAL VAL ILE THR VAL TYR GLU ASP LYS SER PHE
SEQRES 6 B 140 THR PHE ILE ILE LYS THR PRO PRO ALA SER PHE LEU LEU
SEQRES 7 B 140 LYS LYS ALA ALA GLY ILE GLU LYS GLY SER SER GLU PRO
SEQRES 8 B 140 LYS ARG LYS ILE VAL GLY LYS VAL THR ARG LYS GLN ILE
SEQRES 9 B 140 GLU GLU ILE ALA LYS THR LYS MET PRO ASP LEU ASN ALA
SEQRES 10 B 140 ASN SER LEU GLU ALA ALA MET LYS ILE ILE GLU GLY THR
SEQRES 11 B 140 ALA LYS SER MET GLY ILE GLU VAL VAL ASP
SEQRES 1 C 58 G C U G G G A U G U U G G
SEQRES 2 C 58 C U U A G A A G C A G C C
SEQRES 3 C 58 A U C A U U U A A A G A G
SEQRES 4 C 58 U G C G U A A C A G C U C
SEQRES 5 C 58 A C C A G C
SEQRES 1 D 58 G C U G G G A U G U U G G
SEQRES 2 D 58 C U U A G A A G C A G C C
SEQRES 3 D 58 A U C A U U U A A A G A G
SEQRES 4 D 58 U G C G U A A C A G C U C
SEQRES 5 D 58 A C C A G C
HET CD 201 0
HET CD 202 0
HET CD 211 0
HET CD 302 0
HET CD 311 0
HET CD 390 0
HET CD 413 0
HET CD 414 0 SEE REMARK 600
HET MG 210 0
HET MG 214 0
HET MG 215 0
HET MG 223 0
HET MG 225 0
HET MG 226 0
HET MG 228 0
HET MG 257 0
HET MG 273 0
HET MG 318 0
HET MG 326 0
HET MG 354 0
HET MG 360 0
HET MG 365 0
HET MG 375 0

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HET    MG   380      0
HET    MG   385      0
HET    MG   397      0
HET    MG   437      0   SEE REMARK 600
HET    HG   227      0
HET    HG   230      0
HET    HG   332      0
HET    HG   347      0
HET    HG   415      0
HET    HG   416      0
HET    HG   448      0
HET    HG   451      0   SEE REMARK 600
HETNAM     CD CD
HETNAM     MG MG
HETNAM     HG MMC
HETSYN     CD CADMIUM (II)
HETSYN     MG MAGNESIUM (II)
HETSYN     HG METHYLMERCURY ION
FORMUL  5  CD   8(CD1 2+)
FORMUL  6  MG   19(MG1 2+)
FORMUL  7  HG   8(C1 H3 HG1 1+)
FORMUL  8  HOH  *142(H2 O1)
HELIX   1  1 PRO A  26  GLN A  30  1                          5
HELIX   2  2 ILE A  35  ALA A  47  1                         13
HELIX   3  3 ALA A  75  ALA A  83  1                          9
HELIX   4  4 ARG A 102  ASP A 115  1                         14
HELIX   5  5 LEU A 121  SER A 134  1                         14
HELIX   6  6 ALA B  75  ALA B  83  1                          9
HELIX   7  7 ARG B 102  ASP B 115  1                         14
HELIX   8  8 LEU B 121  MET B 135  1                         15
SHEET   1  A 3 ILE A  9  PRO A  14  0
SHEET   2  A 3 ILE A  53  VAL A  60 -1  N  ILE A  58   O  ILE A  9
SHEET   3  A 3 PHE A  66  ILE A  70 -1  N  ILE A  69   O  VAL A  57
SHEET   1  B 2 GLY A  98  THR A 101  0
SHEET   2  B 2 ILE A 137  VAL A 140  1  N  GLU A 138   O  GLY A  98
SHEET   1  C 2 GLY B  98  VAL B 100  0
SHEET   2  C 2 ILE B 137  VAL B 139  1  N  GLU B 138   O  GLY B  98
SITE    1 TSR  2  A C1067   A C1095
SITE    2 TSR  2  A D1067   A D1095
SITE    3 TSR  3 PRO A  22  PRO A  23  PRO A  26
CRYST1  63.890  84.260  155.510  90.00  90.00  90.00 P 21 21 21    8
ORIGX1      1.000000  0.000000  0.000000        0.00000
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
SCALE1      0.015652  0.000000  0.000000        0.00000
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SCALE2      0.000000  0.011868  0.000000        0.00000
SCALE3      0.000000  0.000000  0.006430        0.00000
MTRIX1   1  0.974505  0.101458 -0.200117       -4.54330    1
MTRIX2   1  0.097433 -0.994793 -0.029885       -3.74880    1
MTRIX3   1 -0.202107  0.009626 -0.979316      -50.69290    1
MTRIX1   2  0.973477  0.098780 -0.206364       -4.89630    1
MTRIX2   2  0.098758 -0.995057 -0.010432       -2.89050    1
MTRIX3   2 -0.206374 -0.010225 -0.978420      -50.97240    1
ATOM      1  N   GLN A   8      -7.803 -11.096  -9.783  1.00 71.77      L111 N
ATOM      2  CA  GLN A   8      -8.476  -9.887  -9.223  1.00 79.42      L111 C
ATOM      3  C   GLN A   8      -8.010  -8.599  -9.897  1.00 80.19      L111 C
ATOM      4  O   GLN A   8      -6.857  -8.190  -9.748  1.00 77.92      L111 O
ATOM      5  CB  GLN A   8      -8.212  -9.788  -7.722  1.00 79.86      L111 C
ATOM      6  CG  GLN A   8      -9.065  -8.752  -7.016  1.00 80.16      L111 C
ATOM      7  CD  GLN A   8      -9.072  -8.948  -5.518  1.00 80.58      L111 C
ATOM      8  OE1 GLN A   8      -8.020  -8.963  -4.881  1.00 82.16      L111 O
ATOM      9  NE2 GLN A   8     -10.261  -9.104  -4.946  1.00 79.20      L111 N
ATOM     10  N   ILE A   9      -8.916  -7.963 -10.634  1.00 81.13      L111 N
ATOM     11  CA  ILE A   9      -8.604  -6.723 -11.337  1.00 80.39      L111 C
ATOM     12  C   ILE A   9      -9.312  -5.530 -10.699  1.00 79.13      L111 C
ATOM     13  O   ILE A   9     -10.338  -5.680 -10.036  1.00 78.96      L111 O
ATOM     14  CB  ILE A   9      -9.013  -6.804 -12.834  1.00 77.02      L111 C
ATOM     15  CG1 ILE A   9     -10.534  -6.778 -12.970  1.00 77.57      L111 C
ATOM     16  CG2 ILE A   9      -8.482  -8.080 -13.452  1.00 74.06      L111 C
ATOM     17  CD1 ILE A   9     -11.066  -5.495 -13.552  1.00 83.48      L111 C
ATOM     18  N   LYS A  10      -8.752  -4.343 -10.900  1.00 80.87      L111 N
ATOM     19  CA  LYS A  10      -9.330  -3.121 -10.360  1.00 77.55      L111 C
ATOM     20  C   LYS A  10      -9.252  -2.011 -11.400  1.00 74.90      L111 C
ATOM     21  O   LYS A  10      -8.308  -1.945 -12.191  1.00 69.61      L111 O
ATOM     22  CB  LYS A  10      -8.590  -2.696  -9.089  1.00 78.72      L111 C
ATOM     23  CG  LYS A  10      -7.080  -2.607  -9.243  1.00 76.53      L111 C
ATOM     24  CD  LYS A  10      -6.482  -1.615  -8.256  1.00 76.55      L111 C
ATOM     25  CE  LYS A  10      -6.047  -2.300  -6.968  1.00 78.93      L111 C
ATOM     26  NZ  LYS A  10      -4.923  -1.584  -6.296  1.00 81.54      L111 N
ATOM     27  N   LEU A  11     -10.261  -1.149 -11.403  1.00 72.26      L111 N
ATOM     28  CA  LEU A  11     -10.311  -0.037 -12.342  1.00 77.13      L111 C
ATOM     29  C   LEU A  11     -11.286   1.024 -11.852  1.00 78.99      L111 C
ATOM     30  O   LEU A  11     -12.052   0.790 -10.915  1.00 78.52      L111 O
ATOM     31  CB  LEU A  11     -10.744  -0.525 -13.728  1.00 77.54      L111 C
ATOM     32  CG  LEU A  11     -11.051  -2.014 -13.906  1.00 72.58      L111 C
ATOM     33  CD1 LEU A  11     -12.511  -2.199 -14.290  1.00 68.73      L111 C
ATOM     34  CD2 LEU A  11     -10.128  -2.590 -14.969  1.00 73.75      L111 C
ATOM     35  N   GLN A  12     -11.255   2.189 -12.489  1.00 80.79      L111 N
ATOM     36  CA  GLN A  12     -12.144   3.284 -12.120  1.00 82.10      L111 C
ATOM     37  C   GLN A  12     -13.115   3.582 -13.261  1.00 80.51      L111 C
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ATOM     38  O   GLN A  12     -12.791   4.320 -14.190  1.00 81.39      L111 O
ATOM     39  CB  GLN A  12     -11.329   4.536 -11.789  1.00 81.65      L111 C
ATOM     40  CG  GLN A  12     -10.068   4.267 -10.979  1.00 81.34      L111 C
ATOM     41  CD  GLN A  12      -9.364   5.545 -10.556  1.00 88.15      L111 C
ATOM     42  OE1 GLN A  12      -9.445   6.568 -11.239  1.00 89.05      L111 O
ATOM     43  NE2 GLN A  12      -8.668   5.493  -9.425  1.00 90.09      L111 N
ATOM     44  N   LEU A  13     -14.308   3.003 -13.184  1.00 80.02      L111 N
ATOM     45  CA  LEU A  13     -15.320   3.197 -14.214  1.00 79.90      L111 C
ATOM     46  C   LEU A  13     -16.345   4.256 -13.818  1.00 81.60      L111 C
ATOM     47  O   LEU A  13     -16.761   4.331 -12.659  1.00 82.22      L111 O
ATOM     48  CB  LEU A  13     -16.033   1.873 -14.502  1.00 73.75      L111 C
ATOM     49  CG  LEU A  13     -15.191   0.615 -14.276  1.00 73.16      L111 C
ATOM     50  CD1 LEU A  13     -16.100  -0.586 -14.059  1.00 74.99      L111 C
ATOM     51  CD2 LEU A  13     -14.277   0.397 -15.470  1.00 68.58      L111 C
ATOM     52  N   PRO A  14     -16.759   5.097 -14.783  1.00 80.42      L111 N
ATOM     53  CA  PRO A  14     -17.745   6.151 -14.511  1.00 76.54      L111 C
ATOM     54  C   PRO A  14     -19.065   5.553 -14.041  1.00 74.17      L111 C
ATOM     55  O   PRO A  14     -19.364   4.396 -14.328  1.00 73.53      L111 O
ATOM     56  CB  PRO A  14     -17.877   6.880 -15.846  1.00 74.99      L111 C
ATOM     57  CG  PRO A  14     -17.358   5.919 -16.870  1.00 77.83      L111 C
ATOM     58  CD  PRO A  14     -16.315   5.101 -16.188  1.00 76.88      L111 C
ATOM     59  N   ALA A  15     -19.844   6.349 -13.317  1.00 75.75      L111 N
ATOM     60  CA  ALA A  15     -21.128   5.917 -12.774  1.00 82.83      L111 C
ATOM     61  C   ALA A  15     -21.947   5.008 -13.691  1.00 89.65      L111 C
ATOM     62  O   ALA A  15     -21.711   3.800 -13.753  1.00 93.73      L111 O
ATOM     63  CB  ALA A  15     -21.947   7.132 -12.387  1.00 88.09      L111 C
ATOM     64  N   GLY A  16     -22.921   5.590 -14.387  1.00 94.26      L111 N
ATOM     65  CA  GLY A  16     -23.761   4.810 -15.282  1.00 98.24      L111 C
ATOM     66  C   GLY A  16     -23.218   4.696 -16.697  1.00100.00      L111 C
ATOM     67  O   GLY A  16     -23.672   5.395 -17.607  1.00100.00      L111 O
ATOM     68  N   LYS A  17     -22.239   3.813 -16.881  1.00 99.48      L111 N
ATOM     69  CA  LYS A  17     -21.621   3.594 -18.187  1.00 98.41      L111 C
ATOM     70  C   LYS A  17     -20.588   2.467 -18.117  1.00 99.13      L111 C
ATOM     71  O   LYS A  17     -19.851   2.351 -17.134  1.00100.00      L111 O
ATOM     72  CB  LYS A  17     -20.951   4.883 -18.685  1.00 94.26      L111 C
ATOM     73  CG  LYS A  17     -20.492   5.822 -17.580  1.00 96.55      L111 C
ATOM     74  CD  LYS A  17     -21.088   7.220 -17.728  1.00 97.02      L111 C
ATOM     75  CE  LYS A  17     -21.564   7.773 -16.385  1.00 96.31      L111 C
ATOM     76  NZ  LYS A  17     -20.459   8.345 -15.556  1.00 90.28      L111 N
ATOM     77  N   ALA A  18     -20.545   1.642 -19.163  1.00 98.71      L111 N
ATOM     78  CA  ALA A  18     -19.615   0.517 -19.243  1.00 96.77      L111 C
ATOM     79  C   ALA A  18     -19.707  -0.148 -20.614  1.00 96.63      L111 C
ATOM     80  O   ALA A  18     -20.502   0.271 -21.453  1.00 98.42      L111 O
ATOM     81  CB  ALA A  18     -19.932  -0.500 -18.152  1.00 95.01      L111 C
ATOM     82  N   THR A  19     -18.872  -1.165 -20.837  1.00 96.19      L111 N
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ATOM	83	CA	THR	A	19	-18.843	-1.936	-22.089	1.00 98.62	L111	C
ATOM	84	C	THR	A	19	-17.834	-1.538	-23.177	1.00 98.30	L111	C
ATOM	85	O	THR	A	19	-17.439	-2.379	-23.987	1.00 94.28	L111	O
ATOM	86	CB	THR	A	19	-20.250	-2.000	-22.756	1.00100.00	L111	C
ATOM	87	OG1	THR	A	19	-21.255	-2.212	-21.753	1.00100.00	L111	O
ATOM	88	CG2	THR	A	19	-20.311	-3.135	-23.772	1.00 99.76	L111	C
ATOM	89	N	PRO	A	20	-17.392	-0.267	-23.212	1.00100.00	L111	N
ATOM	90	CA	PRO	A	20	-16.433	0.087	-24.268	1.00100.00	L111	C
ATOM	91	C	PRO	A	20	-15.174	-0.778	-24.289	1.00100.00	L111	C
ATOM	92	O	PRO	A	20	-14.692	-1.220	-23.246	1.00100.00	L111	O
ATOM	93	CB	PRO	A	20	-16.117	1.561	-23.995	1.00100.00	L111	C
ATOM	94	CG	PRO	A	20	-16.510	1.782	-22.568	1.00100.00	L111	C
ATOM	95	CD	PRO	A	20	-17.690	0.887	-22.347	1.00100.00	L111	C
ATOM	96	N	ALA	A	21	-14.650	-1.015	-25.487	1.00100.00	L111	N
ATOM	97	CA	ALA	A	21	-13.450	-1.823	-25.640	1.00100.00	L111	C
ATOM	98	C	ALA	A	21	-12.238	-1.115	-25.030	1.00100.00	L111	C
ATOM	99	O	ALA	A	21	-11.622	-1.626	-24.097	1.00100.00	L111	O
ATOM	100	CB	ALA	A	21	-13.204	-2.130	-27.121	1.00100.00	L111	C
ATOM	101	N	PRO	A	22	-11.886	0.079	-25.542	1.00100.00	L111	N
ATOM	102	CA	PRO	A	22	-10.725	0.773	-24.969	1.00100.00	L111	C
ATOM	103	C	PRO	A	22	-10.740	0.904	-23.434	1.00100.00	L111	C
ATOM	104	O	PRO	A	22	-9.793	0.478	-22.768	1.00100.00	L111	O
ATOM	105	CB	PRO	A	22	-10.726	2.127	-25.683	1.00100.00	L111	C
ATOM	106	CG	PRO	A	22	-11.439	1.862	-26.979	1.00100.00	L111	C
ATOM	107	CD	PRO	A	22	-12.496	0.845	-26.645	1.00100.00	L111	C
ATOM	108	N	PRO	A	23	-11.807	1.495	-22.853	1.00100.00	L111	N
ATOM	109	CA	PRO	A	23	-11.880	1.650	-21.390	1.00100.00	L111	C
ATOM	110	C	PRO	A	23	-11.941	0.338	-20.592	1.00100.00	L111	C
ATOM	111	O	PRO	A	23	-11.025	0.026	-19.829	1.00100.00	L111	O
ATOM	112	CB	PRO	A	23	-13.135	2.507	-21.173	1.00 99.53	L111	C
ATOM	113	CG	PRO	A	23	-13.446	3.100	-22.519	1.00100.00	L111	C
ATOM	114	CD	PRO	A	23	-12.988	2.077	-23.513	1.00100.00	L111	C
ATOM	115	N	VAL	A	24	-13.020	-0.423	-20.767	1.00100.00	L111	N
ATOM	116	CA	VAL	A	24	-13.199	-1.689	-20.051	1.00 95.98	L111	C
ATOM	117	C	VAL	A	24	-12.711	-2.903	-20.844	1.00 94.54	L111	C
ATOM	118	O	VAL	A	24	-11.538	-3.272	-20.773	1.00 88.41	L111	O
ATOM	119	CB	VAL	A	24	-14.688	-1.923	-19.689	1.00 92.89	L111	C
ATOM	120	CG1	VAL	A	24	-14.809	-2.320	-18.232	1.00 90.90	L111	C
ATOM	121	CG2	VAL	A	24	-15.504	-0.668	-19.969	1.00 91.81	L111	C
ATOM	122	N	GLY	A	25	-13.636	-3.515	-21.584	1.00 95.43	L111	N
ATOM	123	CA	GLY	A	25	-13.343	-4.683	-22.401	1.00 94.07	L111	C
ATOM	124	C	GLY	A	25	-11.973	-5.312	-22.224	1.00 94.21	L111	C
ATOM	125	O	GLY	A	25	-11.738	-6.020	-21.243	1.00 93.12	L111	O
ATOM	126	N	PRO	A	26	-11.051	-5.081	-23.176	1.00 93.73	L111	N
ATOM	127	CA	PRO	A	26	-9.684	-5.606	-23.165	1.00 93.06	L111	C

ATOM	128	C	PRO	A	26	-9.110	-5.852	-21.774	1.00	94.47	L111	C
ATOM	129	O	PRO	A	26	-8.633	-6.947	-21.480	1.00	96.39	L111	O
ATOM	130	CB	PRO	A	26	-8.893	-4.546	-23.929	1.00	91.97	L111	C
ATOM	131	CG	PRO	A	26	-9.909	-3.882	-24.840	1.00	86.86	L111	C
ATOM	132	CD	PRO	A	26	-11.299	-4.278	-24.385	1.00	89.82	L111	C
ATOM	133	N	ALA	A	27	-9.167	-4.829	-20.927	1.00	95.87	L111	N
ATOM	134	CA	ALA	A	27	-8.647	-4.902	-19.561	1.00	96.04	L111	C
ATOM	135	C	ALA	A	27	-8.916	-6.234	-18.858	1.00	93.76	L111	C
ATOM	136	O	ALA	A	27	-8.098	-7.152	-18.912	1.00	89.80	L111	O
ATOM	137	CB	ALA	A	27	-9.218	-3.755	-18.730	1.00	98.77	L111	C
ATOM	138	N	LEU	A	28	-10.057	-6.326	-18.185	1.00	92.88	L111	N
ATOM	139	CA	LEU	A	28	-10.424	-7.543	-17.473	1.00	92.03	L111	C
ATOM	140	C	LEU	A	28	-10.935	-8.593	-18.454	1.00	91.54	L111	C
ATOM	141	O	LEU	A	28	-10.992	-9.782	-18.137	1.00	91.91	L111	O
ATOM	142	CB	LEU	A	28	-11.495	-7.237	-16.422	1.00	92.11	L111	C
ATOM	143	CG	LEU	A	28	-12.912	-6.897	-16.898	1.00	91.83	L111	C
ATOM	144	CD1	LEU	A	28	-13.728	-6.405	-15.711	1.00	87.53	L111	C
ATOM	145	CD2	LEU	A	28	-12.870	-5.837	-17.996	1.00	89.79	L111	C
ATOM	146	N	GLY	A	29	-11.304	-8.143	-19.650	1.00	90.13	L111	N
ATOM	147	CA	GLY	A	29	-11.794	-9.060	-20.661	1.00	88.78	L111	C
ATOM	148	C	GLY	A	29	-10.732	-10.074	-21.044	1.00	88.80	L111	C
ATOM	149	O	GLY	A	29	-11.022	-11.064	-21.716	1.00	86.10	L111	O
ATOM	150	N	GLN	A	30	-9.497	-9.826	-20.616	1.00	89.64	L111	N
ATOM	151	CA	GLN	A	30	-8.389	-10.726	-20.919	1.00	91.11	L111	C
ATOM	152	C	GLN	A	30	-7.986	-11.569	-19.712	1.00	91.31	L111	C
ATOM	153	O	GLN	A	30	-6.980	-12.277	-19.747	1.00	89.05	L111	O
ATOM	154	CB	GLN	A	30	-7.177	-9.932	-21.439	1.00	92.85	L111	C
ATOM	155	CG	GLN	A	30	-6.545	-8.965	-20.440	1.00	90.47	L111	C
ATOM	156	CD	GLN	A	30	-5.431	-8.119	-21.055	1.00	92.62	L111	C
ATOM	157	OE1	GLN	A	30	-4.260	-8.511	-21.057	1.00	93.46	L111	O
ATOM	158	NE2	GLN	A	30	-5.796	-6.955	-21.584	1.00	92.21	L111	N
ATOM	159	N	HIS	A	31	-8.776	-11.489	-18.646	1.00	94.67	L111	N
ATOM	160	CA	HIS	A	31	-8.505	-12.256	-17.432	1.00	94.53	L111	C
ATOM	161	C	HIS	A	31	-9.521	-13.393	-17.329	1.00	93.97	L111	C
ATOM	162	O	HIS	A	31	-9.323	-14.351	-16.582	1.00	94.95	L111	O
ATOM	163	CB	HIS	A	31	-8.594	-11.350	-16.193	1.00	92.77	L111	C
ATOM	164	CG	HIS	A	31	-7.423	-10.425	-16.028	1.00	90.32	L111	C
ATOM	165	ND1	HIS	A	31	-7.531	-9.056	-16.160	1.00	88.08	L111	N
ATOM	166	CD2	HIS	A	31	-6.126	-10.671	-15.729	1.00	86.03	L111	C
ATOM	167	CE1	HIS	A	31	-6.351	-8.500	-15.950	1.00	81.34	L111	C
ATOM	168	NE2	HIS	A	31	-5.480	-9.457	-15.686	1.00	84.77	L111	N
ATOM	169	N	GLY	A	32	-10.604	-13.278	-18.094	1.00	93.26	L111	N
ATOM	170	CA	GLY	A	32	-11.637	-14.299	-18.091	1.00	90.69	L111	C
ATOM	171	C	GLY	A	32	-13.032	-13.721	-17.950	1.00	90.58	L111	C
ATOM	172	O	GLY	A	32	-14.022	-14.353	-18.323	1.00	91.06	L111	O

ATOM	173	N	VAL	A	33	-13.107	-12.509	-17.415	1.00 89.92	L111 N
ATOM	174	CA	VAL	A	33	-14.376	-11.822	-17.196	1.00 90.50	L111 C
ATOM	175	C	VAL	A	33	-15.254	-11.711	-18.443	1.00 88.55	L111 C
ATOM	176	O	VAL	A	33	-14.753	-11.581	-19.560	1.00 88.34	L111 O
ATOM	177	CB	VAL	A	33	-14.135	-10.398	-16.652	1.00 92.08	L111 C
ATOM	178	CG1	VAL	A	33	-15.292	-9.976	-15.770	1.00 90.59	L111 C
ATOM	179	CG2	VAL	A	33	-12.830	-10.351	-15.873	1.00 93.31	L111 C
ATOM	180	N	ASN	A	34	-16.568	-11.766	-18.237	1.00 89.80	L111 N
ATOM	181	CA	ASN	A	34	-17.533	-11.650	-19.327	1.00 94.89	L111 C
ATOM	182	C	ASN	A	34	-18.128	-10.245	-19.290	1.00 96.48	L111 C
ATOM	183	O	ASN	A	34	-19.141	-10.008	-18.630	1.00 97.04	L111 O
ATOM	184	CB	ASN	A	34	-18.661	-12.681	-19.182	1.00 97.83	L111 C
ATOM	185	CG	ASN	A	34	-18.405	-13.683	-18.072	1.00100.00	L111 C
ATOM	186	OD1	ASN	A	34	-19.205	-13.813	-17.141	1.00100.00	L111 O
ATOM	187	ND2	ASN	A	34	-17.291	-14.405	-18.167	1.00100.00	L111 N
ATOM	188	N	ILE	A	35	-17.486	-9.325	-20.006	1.00 98.20	L111 N
ATOM	189	CA	ILE	A	35	-17.898	-7.922	-20.071	1.00 97.32	L111 C
ATOM	190	C	ILE	A	35	-19.392	-7.651	-19.844	1.00 99.75	L111 C
ATOM	191	O	ILE	A	35	-19.776	-7.148	-18.788	1.00100.00	L111 O
ATOM	192	CB	ILE	A	35	-17.478	-7.282	-21.426	1.00 95.15	L111 C
ATOM	193	CG1	ILE	A	35	-16.341	-8.094	-22.064	1.00 93.73	L111 C
ATOM	194	CG2	ILE	A	35	-17.066	-5.823	-21.213	1.00 87.68	L111 C
ATOM	195	CD1	ILE	A	35	-14.960	-7.824	-21.485	1.00 91.66	L111 C
ATOM	196	N	MET	A	36	-20.220	-7.980	-20.835	1.00100.00	L111 N
ATOM	197	CA	MET	A	36	-21.672	-7.767	-20.773	1.00 99.82	L111 C
ATOM	198	C	MET	A	36	-22.294	-7.868	-19.376	1.00 97.54	L111 C
ATOM	199	O	MET	A	36	-23.032	-6.975	-18.950	1.00 95.12	L111 O
ATOM	200	CB	MET	A	36	-22.384	-8.752	-21.713	1.00100.00	L111 C
ATOM	201	CG	MET	A	36	-23.911	-8.645	-21.709	1.00100.00	L111 C
ATOM	202	SD	MET	A	36	-24.759	-10.248	-21.810	1.00100.00	L111 S
ATOM	203	CE	MET	A	36	-25.601	-10.300	-20.213	1.00 97.00	L111 C
ATOM	204	N	GLU	A	37	-22.001	-8.960	-18.674	1.00 95.35	L111 N
ATOM	205	CA	GLU	A	37	-22.535	-9.190	-17.335	1.00 92.68	L111 C
ATOM	206	C	GLU	A	37	-22.124	-8.100	-16.349	1.00 93.66	L111 C
ATOM	207	O	GLU	A	37	-22.925	-7.672	-15.515	1.00 91.34	L111 O
ATOM	208	CB	GLU	A	37	-22.071	-10.552	-16.819	1.00 90.67	L111 C
ATOM	209	CG	GLU	A	37	-23.205	-11.512	-16.511	1.00 93.38	L111 C
ATOM	210	CD	GLU	A	37	-22.929	-12.372	-15.290	1.00 96.55	L111 C
ATOM	211	OE1	GLU	A	37	-22.044	-13.254	-15.365	1.00 91.81	L111 O
ATOM	212	OE2	GLU	A	37	-23.600	-12.163	-14.256	1.00 99.15	L111 O
ATOM	213	N	PHE	A	38	-20.872	-7.657	-16.449	1.00 94.99	L111 N
ATOM	214	CA	PHE	A	38	-20.335	-6.614	-15.575	1.00 95.14	L111 C
ATOM	215	C	PHE	A	38	-20.928	-5.243	-15.907	1.00 93.32	L111 C
ATOM	216	O	PHE	A	38	-21.382	-4.527	-15.017	1.00 92.65	L111 O
ATOM	217	CB	PHE	A	38	-18.802	-6.565	-15.693	1.00 93.51	L111 C

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ATOM   218  CG  PHE A  38     -18.139  -5.586 -14.748  1.00 96.97      L111 C
ATOM   219  CD1 PHE A  38     -18.716  -5.269 -13.518  1.00 98.99      L111 C
ATOM   220  CD2 PHE A  38     -16.935  -4.978 -15.094  1.00 96.40      L111 C
ATOM   221  CE1 PHE A  38     -18.106  -4.355 -12.651  1.00 95.25      L111 C
ATOM   222  CE2 PHE A  38     -16.318  -4.064 -14.233  1.00 96.95      L111 C
ATOM   223  CZ  PHE A  38     -16.905  -3.754 -13.010  1.00 92.93      L111 C
ATOM   224  N   CYS A  39     -20.925  -4.884 -17.187  1.00 94.43      L111 N
ATOM   225  CA  CYS A  39     -21.461  -3.597 -17.632  1.00 95.64      L111 C
ATOM   226  C   CYS A  39     -22.840  -3.321 -17.044  1.00 96.32      L111 C
ATOM   227  O   CYS A  39     -23.051  -2.295 -16.392  1.00 95.48      L111 O
ATOM   228  CB  CYS A  39     -21.540  -3.563 -19.159  1.00 93.89      L111 C
ATOM   229  SG  CYS A  39     -19.986  -3.992 -19.971  1.00100.00      L111 S
ATOM   230  N   LYS A  40     -23.774  -4.239 -17.279  1.00 96.81      L111 N
ATOM   231  CA  LYS A  40     -25.133  -4.101 -16.768  1.00 96.22      L111 C
ATOM   232  C   LYS A  40     -25.135  -4.168 -15.240  1.00 95.74      L111 C
ATOM   233  O   LYS A  40     -25.823  -3.389 -14.576  1.00 96.26      L111 O
ATOM   234  CB  LYS A  40     -26.029  -5.205 -17.339  1.00 95.66      L111 C
ATOM   235  CG  LYS A  40     -25.956  -5.344 -18.855  1.00 97.68      L111 C
ATOM   236  CD  LYS A  40     -27.132  -6.148 -19.401  1.00 95.99      L111 C
ATOM   237  CE  LYS A  40     -26.947  -6.475 -20.880  1.00 94.18      L111 C
ATOM   238  NZ  LYS A  40     -28.171  -6.189 -21.684  1.00 88.70      L111 N
ATOM   239  N   ARG A  41     -24.356  -5.097 -14.688  1.00 92.53      L111 N
ATOM   240  CA  ARG A  41     -24.262  -5.260 -13.239  1.00 89.97      L111 C
ATOM   241  C   ARG A  41     -23.694  -4.003 -12.582  1.00 90.13      L111 C
ATOM   242  O   ARG A  41     -24.306  -3.433 -11.679  1.00 91.63      L111 O
ATOM   243  CB  ARG A  41     -23.375  -6.459 -12.900  1.00 85.72      L111 C
ATOM   244  CG  ARG A  41     -24.143  -7.710 -12.526  1.00 85.51      L111 C
ATOM   245  CD  ARG A  41     -23.330  -8.594 -11.595  1.00 90.22      L111 C
ATOM   246  NE  ARG A  41     -22.610  -9.641 -12.318  1.00 88.90      L111 N
ATOM   247  CZ  ARG A  41     -21.670 -10.412 -11.778  1.00 87.28      L111 C
ATOM   248  NH1 ARG A  41     -21.332 -10.257 -10.501  1.00 84.21      L111 N
ATOM   249  NH2 ARG A  41     -21.070 -11.340 -12.511  1.00 80.87      L111 N
ATOM   250  N   PHE A  42     -22.517  -3.583 -13.037  1.00 87.95      L111 N
ATOM   251  CA  PHE A  42     -21.865  -2.393 -12.509  1.00 82.17      L111 C
ATOM   252  C   PHE A  42     -22.838  -1.228 -12.587  1.00 83.84      L111 C
ATOM   253  O   PHE A  42     -23.215  -0.648 -11.566  1.00 84.64      L111 O
ATOM   254  CB  PHE A  42     -20.608  -2.074 -13.325  1.00 78.71      L111 C
ATOM   255  CG  PHE A  42     -19.934  -0.792 -12.925  1.00 83.84      L111 C
ATOM   256  CD1 PHE A  42     -19.109  -0.745 -11.802  1.00 84.59      L111 C
ATOM   257  CD2 PHE A  42     -20.132   0.373 -13.662  1.00 83.65      L111 C
ATOM   258  CE1 PHE A  42     -18.490   0.444 -11.417  1.00 79.21      L111 C
ATOM   259  CE2 PHE A  42     -19.518   1.567 -13.289  1.00 77.97      L111 C
ATOM   260  CZ  PHE A  42     -18.695   1.602 -12.162  1.00 81.55      L111 C
ATOM   261  N   ASN A  43     -23.253  -0.906 -13.808  1.00 85.30      L111 N
ATOM   262  CA  ASN A  43     -24.181   0.191 -14.053  1.00 86.52      L111 C
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ATOM  263  C   ASN A  43     -25.488   0.062 -13.284  1.00 85.43      L111 C
ATOM  264  O   ASN A  43     -26.281   1.000 -13.240  1.00 85.51      L111 O
ATOM  265  CB  ASN A  43     -24.476   0.296 -15.548  1.00 86.27      L111 C
ATOM  266  CG  ASN A  43     -23.265   0.716 -16.344  1.00 92.38      L111 C
ATOM  267  OD1 ASN A  43     -22.347   1.340 -15.811  1.00 96.74      L111 O
ATOM  268  ND2 ASN A  43     -23.249   0.374 -17.627  1.00 99.06      L111 N
ATOM  269  N   ALA A  44     -25.712  -1.098 -12.679  1.00 85.49      L111 N
ATOM  270  CA  ALA A  44     -26.930  -1.319 -11.912  1.00 84.79      L111 C
ATOM  271  C   ALA A  44     -26.900  -0.515 -10.618  1.00 85.21      L111 C
ATOM  272  O   ALA A  44     -27.668   0.433 -10.452  1.00 84.84      L111 O
ATOM  273  CB  ALA A  44     -27.092  -2.797 -11.603  1.00 86.85      L111 C
ATOM  274  N   GLU A  45     -26.005  -0.893  -9.708  1.00 85.98      L111 N
ATOM  275  CA  GLU A  45     -25.885  -0.211  -8.420  1.00 90.10      L111 C
ATOM  276  C   GLU A  45     -25.222   1.158  -8.536  1.00 89.46      L111 C
ATOM  277  O   GLU A  45     -25.388   2.010  -7.661  1.00 88.02      L111 O
ATOM  278  CB  GLU A  45     -25.103  -1.076  -7.427  1.00 89.91      L111 C
ATOM  279  CG  GLU A  45     -23.812  -1.641  -7.983  1.00 93.26      L111 C
ATOM  280  CD  GLU A  45     -23.917  -3.118  -8.293  1.00 95.55      L111 C
ATOM  281  OE1 GLU A  45     -24.558  -3.844  -7.503  1.00 94.41      L111 O
ATOM  282  OE2 GLU A  45     -23.360  -3.551  -9.326  1.00 98.04      L111 O
ATOM  283  N   THR A  46     -24.463   1.369  -9.608  1.00 89.00      L111 N
ATOM  284  CA  THR A  46     -23.806   2.655  -9.810  1.00 91.97      L111 C
ATOM  285  C   THR A  46     -24.849   3.680 -10.261  1.00 95.20      L111 C
ATOM  286  O   THR A  46     -24.516   4.737 -10.806  1.00 95.92      L111 O
ATOM  287  CB  THR A  46     -22.681   2.560 -10.865  1.00 90.40      L111 C
ATOM  288  OG1 THR A  46     -23.232   2.170 -12.129  1.00 88.41      L111 O
ATOM  289  CG2 THR A  46     -21.634   1.545 -10.429  1.00 87.67      L111 C
ATOM  290  N   ALA A  47     -26.116   3.343 -10.031  1.00 95.70      L111 N
ATOM  291  CA  ALA A  47     -27.237   4.208 -10.374  1.00 93.30      L111 C
ATOM  292  C   ALA A  47     -27.464   5.142  -9.191  1.00 95.59      L111 C
ATOM  293  O   ALA A  47     -27.681   6.341  -9.367  1.00 97.14      L111 O
ATOM  294  CB  ALA A  47     -28.488   3.373 -10.634  1.00 85.02      L111 C
ATOM  295  N   ASP A  48     -27.409   4.580  -7.985  1.00 98.95      L111 N
ATOM  296  CA  ASP A  48     -27.589   5.360  -6.764  1.00100.00      L111 C
ATOM  297  C   ASP A  48     -26.667   6.582  -6.823  1.00100.00      L111 C
ATOM  298  O   ASP A  48     -27.065   7.697  -6.477  1.00100.00      L111 O
ATOM  299  CB  ASP A  48     -27.248   4.515  -5.526  1.00100.00      L111 C
ATOM  300  CG  ASP A  48     -27.577   3.038  -5.706  1.00100.00      L111 C
ATOM  301  OD1 ASP A  48     -28.633   2.721  -6.297  1.00100.00      L111 O
ATOM  302  OD2 ASP A  48     -26.777   2.191  -5.249  1.00100.00      L111 O
ATOM  303  N   LYS A  49     -25.434   6.356  -7.270  1.00100.00      L111 N
ATOM  304  CA  LYS A  49     -24.440   7.419  -7.394  1.00 99.10      L111 C
ATOM  305  C   LYS A  49     -24.009   7.547  -8.859  1.00 98.06      L111 C
ATOM  306  O   LYS A  49     -23.106   6.842  -9.318  1.00 95.26      L111 O
ATOM  307  CB  LYS A  49     -23.226   7.105  -6.512  1.00 94.97      L111 C
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ATOM	308	CG	LYS	A	49	-23.561	6.908	-5.037	1.00	92.57	L111 C
ATOM	309	CD	LYS	A	49	-22.956	5.619	-4.498	1.00	93.51	L111 C
ATOM	310	CE	LYS	A	49	-21.611	5.873	-3.827	1.00	94.40	L111 C
ATOM	311	NZ	LYS	A	49	-20.528	4.998	-4.365	1.00	88.97	L111 N
ATOM	312	N	ALA	A	50	-24.661	8.450	-9.587	1.00	95.33	L111 N
ATOM	313	CA	ALA	A	50	-24.360	8.653	-10.999	1.00	93.02	L111 C
ATOM	314	C	ALA	A	50	-23.680	9.985	-11.305	1.00	91.25	L111 C
ATOM	315	O	ALA	A	50	-23.898	10.986	-10.619	1.00	90.14	L111 O
ATOM	316	CB	ALA	A	50	-25.636	8.522	-11.819	1.00	96.51	L111 C
ATOM	317	N	GLY	A	51	-22.861	9.984	-12.353	1.00	89.39	L111 N
ATOM	318	CA	GLY	A	51	-22.153	11.186	-12.752	1.00	90.09	L111 C
ATOM	319	C	GLY	A	51	-20.709	11.173	-12.289	1.00	91.40	L111 C
ATOM	320	O	GLY	A	51	-19.828	11.733	-12.943	1.00	91.06	L111 O
ATOM	321	N	MET	A	52	-20.465	10.520	-11.158	1.00	91.81	L111 N
ATOM	322	CA	MET	A	52	-19.125	10.440	-10.591	1.00	88.05	L111 C
ATOM	323	C	MET	A	52	-18.347	9.218	-11.062	1.00	84.95	L111 C
ATOM	324	O	MET	A	52	-18.927	8.206	-11.455	1.00	85.89	L111 O
ATOM	325	CB	MET	A	52	-19.207	10.425	-9.065	1.00	85.66	L111 C
ATOM	326	CG	MET	A	52	-20.358	11.236	-8.503	1.00	86.98	L111 C
ATOM	327	SD	MET	A	52	-20.028	11.840	-6.840	1.00	94.43	L111 S
ATOM	328	CE	MET	A	52	-18.414	12.577	-7.060	1.00	92.32	L111 C
ATOM	329	N	ILE	A	53	-17.025	9.330	-11.021	1.00	80.70	L111 N
ATOM	330	CA	ILE	A	53	-16.145	8.242	-11.415	1.00	76.40	L111 C
ATOM	331	C	ILE	A	53	-15.856	7.437	-10.157	1.00	76.01	L111 C
ATOM	332	O	ILE	A	53	-15.214	7.937	-9.238	1.00	80.34	L111 O
ATOM	333	CB	ILE	A	53	-14.815	8.781	-11.987	1.00	72.67	L111 C
ATOM	334	CG1	ILE	A	53	-15.035	9.279	-13.421	1.00	73.66	L111 C
ATOM	335	CG2	ILE	A	53	-13.735	7.706	-11.897	1.00	69.87	L111 C
ATOM	336	CD1	ILE	A	53	-14.073	8.712	-14.461	1.00	67.81	L111 C
ATOM	337	N	LEU	A	54	-16.337	6.199	-10.110	1.00	77.62	L111 N
ATOM	338	CA	LEU	A	54	-16.123	5.355	-8.940	1.00	75.31	L111 C
ATOM	339	C	LEU	A	54	-15.263	4.129	-9.242	1.00	73.26	L111 C
ATOM	340	O	LEU	A	54	-15.468	3.448	-10.248	1.00	69.71	L111 O
ATOM	341	CB	LEU	A	54	-17.471	4.913	-8.354	1.00	74.18	L111 C
ATOM	342	CG	LEU	A	54	-18.446	4.186	-9.283	1.00	76.71	L111 C
ATOM	343	CD1	LEU	A	54	-19.398	3.339	-8.456	1.00	78.50	L111 C
ATOM	344	CD2	LEU	A	54	-19.221	5.196	-10.112	1.00	77.50	L111 C
ATOM	345	N	PRO	A	55	-14.277	3.841	-8.368	1.00	73.50	L111 N
ATOM	346	CA	PRO	A	55	-13.379	2.694	-8.531	1.00	73.63	L111 C
ATOM	347	C	PRO	A	55	-13.998	1.397	-8.010	1.00	72.99	L111 C
ATOM	348	O	PRO	A	55	-14.516	1.349	-6.895	1.00	76.87	L111 O
ATOM	349	CB	PRO	A	55	-12.139	3.096	-7.736	1.00	69.02	L111 C
ATOM	350	CG	PRO	A	55	-12.654	4.000	-6.669	1.00	66.68	L111 C
ATOM	351	CD	PRO	A	55	-13.950	4.617	-7.157	1.00	72.43	L111 C
ATOM	352	N	VAL	A	56	-13.945	0.349	-8.825	1.00	70.25	L111 N

ATOM	353	CA	VAL	A	56	-14.496	-0.942	-8.440	1.00	70.19	L111	C
ATOM	354	C	VAL	A	56	-13.399	-1.999	-8.486	1.00	70.07	L111	C
ATOM	355	O	VAL	A	56	-12.502	-1.937	-9.329	1.00	67.23	L111	O
ATOM	356	CB	VAL	A	56	-15.654	-1.361	-9.384	1.00	67.10	L111	C
ATOM	357	CG1	VAL	A	56	-15.246	-1.161	-10.828	1.00	67.75	L111	C
ATOM	358	CG2	VAL	A	56	-16.034	-2.808	-9.143	1.00	62.26	L111	C
ATOM	359	N	VAL	A	57	-13.459	-2.956	-7.565	1.00	72.09	L111	N
ATOM	360	CA	VAL	A	57	-12.472	-4.027	-7.527	1.00	73.93	L111	C
ATOM	361	C	VAL	A	57	-13.121	-5.341	-7.934	1.00	76.94	L111	C
ATOM	362	O	VAL	A	57	-13.788	-6.001	-7.131	1.00	78.31	L111	O
ATOM	363	CB	VAL	A	57	-11.849	-4.189	-6.127	1.00	68.90	L111	C
ATOM	364	CG1	VAL	A	57	-10.940	-5.410	-6.104	1.00	66.82	L111	C
ATOM	365	CG2	VAL	A	57	-11.058	-2.948	-5.767	1.00	67.57	L111	C
ATOM	366	N	ILE	A	58	-12.923	-5.702	-9.197	1.00	79.04	L111	N
ATOM	367	CA	ILE	A	58	-13.467	-6.930	-9.756	1.00	77.59	L111	C
ATOM	368	C	ILE	A	58	-12.611	-8.115	-9.319	1.00	77.59	L111	C
ATOM	369	O	ILE	A	58	-11.383	-8.023	-9.262	1.00	73.20	L111	O
ATOM	370	CB	ILE	A	58	-13.490	-6.863	-11.307	1.00	76.77	L111	C
ATOM	371	CG1	ILE	A	58	-14.689	-6.033	-11.773	1.00	79.34	L111	C
ATOM	372	CG2	ILE	A	58	-13.526	-8.267	-11.904	1.00	73.40	L111	C
ATOM	373	CD1	ILE	A	58	-15.970	-6.832	-11.963	1.00	82.47	L111	C
ATOM	374	N	THR	A	59	-13.270	-9.224	-8.999	1.00	82.32	L111	N
ATOM	375	CA	THR	A	59	-12.581	-10.444	-8.589	1.00	82.77	L111	C
ATOM	376	C	THR	A	59	-13.114	-11.602	-9.430	1.00	83.16	L111	C
ATOM	377	O	THR	A	59	-14.312	-11.888	-9.417	1.00	78.62	L111	O
ATOM	378	CB	THR	A	59	-12.815	-10.761	-7.091	1.00	81.80	L111	C
ATOM	379	OG1	THR	A	59	-12.872	-9.539	-6.341	1.00	79.00	L111	O
ATOM	380	CG2	THR	A	59	-11.682	-11.629	-6.552	1.00	74.95	L111	C
ATOM	381	N	VAL	A	60	-12.221	-12.256	-10.168	1.00	84.63	L111	N
ATOM	382	CA	VAL	A	60	-12.603	-13.377	-11.022	1.00	85.45	L111	C
ATOM	383	C	VAL	A	60	-12.140	-14.723	-10.466	1.00	85.80	L111	C
ATOM	384	O	VAL	A	60	-10.947	-14.934	-10.228	1.00	83.46	L111	O
ATOM	385	CB	VAL	A	60	-12.030	-13.211	-12.445	1.00	85.69	L111	C
ATOM	386	CG1	VAL	A	60	-12.984	-12.383	-13.295	1.00	80.95	L111	C
ATOM	387	CG2	VAL	A	60	-10.653	-12.563	-12.380	1.00	84.62	L111	C
ATOM	388	N	TYR	A	61	-13.098	-15.629	-10.272	1.00	86.41	L111	N
ATOM	389	CA	TYR	A	61	-12.827	-16.965	-9.747	1.00	88.03	L111	C
ATOM	390	C	TYR	A	61	-12.459	-17.915	-10.877	1.00	89.54	L111	C
ATOM	391	O	TYR	A	61	-12.885	-17.721	-12.015	1.00	93.25	L111	O
ATOM	392	CB	TYR	A	61	-14.056	-17.486	-8.998	1.00	87.73	L111	C
ATOM	393	CG	TYR	A	61	-14.589	-16.487	-7.999	1.00	91.62	L111	C
ATOM	394	CD1	TYR	A	61	-13.873	-16.187	-6.837	1.00	89.76	L111	C
ATOM	395	CD2	TYR	A	61	-15.772	-15.788	-8.244	1.00	89.94	L111	C
ATOM	396	CE1	TYR	A	61	-14.316	-15.214	-5.947	1.00	89.76	L111	C
ATOM	397	CE2	TYR	A	61	-16.225	-14.810	-7.358	1.00	92.12	L111	C

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ATOM    398  CZ  TYR A  61     -15.489 -14.526  -6.214  1.00 92.07      L111 C
ATOM    399  OH  TYR A  61     -15.910 -13.543  -5.347  1.00 94.51      L111 O
ATOM    400  N   GLU A  62     -11.666 -18.936 -10.557  1.00 89.59      L111 N
ATOM    401  CA  GLU A  62     -11.218 -19.921 -11.541  1.00 86.30      L111 C
ATOM    402  C   GLU A  62     -12.248 -20.245 -12.626  1.00 84.38      L111 C
ATOM    403  O   GLU A  62     -11.886 -20.480 -13.779  1.00 83.12      L111 O
ATOM    404  CB  GLU A  62     -10.798 -21.217 -10.835  1.00 86.59      L111 C
ATOM    405  CG  GLU A  62     -11.842 -21.781  -9.872  1.00 98.78      L111 C
ATOM    406  CD  GLU A  62     -12.709 -22.865 -10.502  1.00100.00      L111 C
ATOM    407  OE1 GLU A  62     -12.149 -23.866 -11.007  1.00100.00      L111 O
ATOM    408  OE2 GLU A  62     -13.952 -22.711 -10.490  1.00100.00      L111 O
ATOM    409  N   ASP A  63     -13.527 -20.246 -12.261  1.00 83.04      L111 N
ATOM    410  CA  ASP A  63     -14.593 -20.554 -13.210  1.00 83.65      L111 C
ATOM    411  C   ASP A  63     -15.045 -19.360 -14.066  1.00 89.63      L111 C
ATOM    412  O   ASP A  63     -16.153 -19.364 -14.609  1.00 90.46      L111 O
ATOM    413  CB  ASP A  63     -15.795 -21.132 -12.461  1.00 80.07      L111 C
ATOM    414  CG  ASP A  63     -16.738 -20.061 -11.968  1.00 79.27      L111 C
ATOM    415  OD1 ASP A  63     -16.275 -19.146 -11.254  1.00 85.70      L111 O
ATOM    416  OD2 ASP A  63     -17.941 -20.130 -12.298  1.00 76.37      L111 O
ATOM    417  N   LYS A  64     -14.188 -18.347 -14.185  1.00 91.01      L111 N
ATOM    418  CA  LYS A  64     -14.481 -17.150 -14.976  1.00 89.76      L111 C
ATOM    419  C   LYS A  64     -15.585 -16.261 -14.398  1.00 89.42      L111 C
ATOM    420  O   LYS A  64     -15.809 -15.149 -14.882  1.00 91.74      L111 O
ATOM    421  CB  LYS A  64     -14.833 -17.540 -16.418  1.00 92.48      L111 C
ATOM    422  CG  LYS A  64     -13.737 -17.237 -17.436  1.00 92.64      L111 C
ATOM    423  CD  LYS A  64     -12.362 -17.682 -16.936  1.00 89.88      L111 C
ATOM    424  CE  LYS A  64     -11.520 -18.269 -18.060  1.00 87.02      L111 C
ATOM    425  NZ  LYS A  64     -12.331 -18.548 -19.280  1.00 89.34      L111 N
ATOM    426  N   SER A  65     -16.280 -16.748 -13.373  1.00 88.30      L111 N
ATOM    427  CA  SER A  65     -17.336 -15.966 -12.738  1.00 87.60      L111 C
ATOM    428  C   SER A  65     -16.668 -14.827 -11.979  1.00 90.25      L111 C
ATOM    429  O   SER A  65     -15.443 -14.800 -11.857  1.00 94.42      L111 O
ATOM    430  CB  SER A  65     -18.138 -16.830 -11.766  1.00 83.90      L111 C
ATOM    431  OG  SER A  65     -19.255 -16.115 -11.265  1.00 86.12      L111 O
ATOM    432  N   PHE A  66     -17.459 -13.895 -11.456  1.00 89.68      L111 N
ATOM    433  CA  PHE A  66     -16.872 -12.769 -10.737  1.00 86.65      L111 C
ATOM    434  C   PHE A  66     -17.824 -11.963  -9.852  1.00 84.85      L111 C
ATOM    435  O   PHE A  66     -19.049 -12.065  -9.956  1.00 84.96      L111 O
ATOM    436  CB  PHE A  66     -16.207 -11.819 -11.740  1.00 83.79      L111 C
ATOM    437  CG  PHE A  66     -17.166 -11.224 -12.736  1.00 84.15      L111 C
ATOM    438  CD1 PHE A  66     -17.849 -10.044 -12.446  1.00 84.23      L111 C
ATOM    439  CD2 PHE A  66     -17.402 -11.851 -13.955  1.00 85.47      L111 C
ATOM    440  CE1 PHE A  66     -18.756  -9.496 -13.358  1.00 83.49      L111 C
ATOM    441  CE2 PHE A  66     -18.307 -11.312 -14.875  1.00 85.83      L111 C
ATOM    442  CZ  PHE A  66     -18.985 -10.132 -14.574  1.00 81.40      L111 C
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ATOM	443	N	THR	A	67	-17.223	-11.166	-8.975	1.00	83.77	L111	N
ATOM	444	CA	THR	A	67	-17.937	-10.279	-8.065	1.00	79.66	L111	C
ATOM	445	C	THR	A	67	-17.102	-9.009	-8.062	1.00	79.21	L111	C
ATOM	446	O	THR	A	67	-16.005	-8.985	-8.623	1.00	78.86	L111	O
ATOM	447	CB	THR	A	67	-17.990	-10.835	-6.630	1.00	77.12	L111	C
ATOM	448	OG1	THR	A	67	-16.660	-11.101	-6.169	1.00	71.17	L111	O
ATOM	449	CG2	THR	A	67	-18.807	-12.112	-6.585	1.00	76.03	L111	C
ATOM	450	N	PHE	A	68	-17.603	-7.954	-7.439	1.00	77.92	L111	N
ATOM	451	CA	PHE	A	68	-16.850	-6.711	-7.409	1.00	76.33	L111	C
ATOM	452	C	PHE	A	68	-17.396	-5.750	-6.379	1.00	74.52	L111	C
ATOM	453	O	PHE	A	68	-18.609	-5.594	-6.241	1.00	74.74	L111	O
ATOM	454	CB	PHE	A	68	-16.871	-6.046	-8.789	1.00	79.76	L111	C
ATOM	455	CG	PHE	A	68	-18.255	-5.772	-9.311	1.00	78.43	L111	C
ATOM	456	CD1	PHE	A	68	-18.994	-6.781	-9.922	1.00	77.56	L111	C
ATOM	457	CD2	PHE	A	68	-18.821	-4.506	-9.193	1.00	77.06	L111	C
ATOM	458	CE1	PHE	A	68	-20.276	-6.532	-10.409	1.00	79.65	L111	C
ATOM	459	CE2	PHE	A	68	-20.103	-4.247	-9.677	1.00	76.90	L111	C
ATOM	460	CZ	PHE	A	68	-20.831	-5.263	-10.285	1.00	77.56	L111	C
ATOM	461	N	ILE	A	69	-16.491	-5.105	-5.656	1.00	73.94	L111	N
ATOM	462	CA	ILE	A	69	-16.885	-4.142	-4.644	1.00	70.90	L111	C
ATOM	463	C	ILE	A	69	-16.752	-2.736	-5.218	1.00	71.09	L111	C
ATOM	464	O	ILE	A	69	-15.773	-2.420	-5.901	1.00	68.28	L111	O
ATOM	465	CB	ILE	A	69	-16.010	-4.273	-3.377	1.00	65.36	L111	C
ATOM	466	CG1	ILE	A	69	-14.550	-3.966	-3.709	1.00	63.63	L111	C
ATOM	467	CG2	ILE	A	69	-16.119	-5.682	-2.820	1.00	61.98	L111	C
ATOM	468	CD1	ILE	A	69	-13.850	-3.146	-2.650	1.00	54.75	L111	C
ATOM	469	N	ILE	A	70	-17.753	-1.903	-4.962	1.00	68.20	L111	N
ATOM	470	CA	ILE	A	70	-17.740	-0.530	-5.443	1.00	65.88	L111	C
ATOM	471	C	ILE	A	70	-17.350	0.388	-4.283	1.00	61.84	L111	C
ATOM	472	O	ILE	A	70	-17.975	0.367	-3.222	1.00	60.58	L111	O
ATOM	473	CB	ILE	A	70	-19.126	-0.135	-6.022	1.00	66.46	L111	C
ATOM	474	CG1	ILE	A	70	-19.030	-0.026	-7.545	1.00	67.64	L111	C
ATOM	475	CG2	ILE	A	70	-19.608	1.187	-5.432	1.00	69.87	L111	C
ATOM	476	CD1	ILE	A	70	-19.695	-1.163	-8.283	1.00	63.00	L111	C
ATOM	477	N	LYS	A	71	-16.301	1.179	-4.489	1.00	55.49	L111	N
ATOM	478	CA	LYS	A	71	-15.820	2.092	-3.463	1.00	49.56	L111	C
ATOM	479	C	LYS	A	71	-16.181	3.531	-3.773	1.00	51.89	L111	C
ATOM	480	O	LYS	A	71	-16.814	3.826	-4.787	1.00	58.09	L111	O
ATOM	481	CB	LYS	A	71	-14.301	1.996	-3.325	1.00	41.23	L111	C
ATOM	482	CG	LYS	A	71	-13.736	0.617	-3.549	1.00	45.62	L111	C
ATOM	483	CD	LYS	A	71	-12.280	0.573	-3.134	1.00	47.82	L111	C
ATOM	484	CE	LYS	A	71	-12.066	-0.371	-1.962	1.00	53.59	L111	C
ATOM	485	NZ	LYS	A	71	-10.785	-1.130	-2.085	1.00	54.56	L111	N
ATOM	486	N	THR	A	72	-15.763	4.424	-2.883	1.00	51.64	L111	N
ATOM	487	CA	THR	A	72	-16.005	5.851	-3.034	1.00	48.54	L111	C

ATOM	488	C	THR	A	72	-15.040	6.390	-4.088	1.00	47.19	L111	C
ATOM	489	O	THR	A	72	-13.919	5.896	-4.227	1.00	51.43	L111	O
ATOM	490	CB	THR	A	72	-15.758	6.584	-1.711	1.00	49.44	L111	C
ATOM	491	OG1	THR	A	72	-14.374	6.469	-1.356	1.00	56.76	L111	O
ATOM	492	CG2	THR	A	72	-16.598	5.975	-0.602	1.00	49.50	L111	C
ATOM	493	N	PRO	A	73	-15.463	7.409	-4.850	1.00	43.35	L111	N
ATOM	494	CA	PRO	A	73	-14.603	7.989	-5.890	1.00	39.98	L111	C
ATOM	495	C	PRO	A	73	-13.260	8.487	-5.357	1.00	38.40	L111	C
ATOM	496	O	PRO	A	73	-13.153	8.908	-4.206	1.00	41.41	L111	O
ATOM	497	CB	PRO	A	73	-15.449	9.117	-6.483	1.00	40.56	L111	C
ATOM	498	CG	PRO	A	73	-16.536	9.360	-5.490	1.00	44.56	L111	C
ATOM	499	CD	PRO	A	73	-16.775	8.071	-4.781	1.00	42.40	L111	C
ATOM	500	N	PRO	A	74	-12.217	8.453	-6.198	1.00	36.48	L111	N
ATOM	501	CA	PRO	A	74	-10.882	8.904	-5.788	1.00	35.21	L111	C
ATOM	502	C	PRO	A	74	-10.881	10.296	-5.162	1.00	32.68	L111	C
ATOM	503	O	PRO	A	74	-11.778	11.102	-5.406	1.00	30.40	L111	O
ATOM	504	CB	PRO	A	74	-10.066	8.856	-7.082	1.00	37.87	L111	C
ATOM	505	CG	PRO	A	74	-10.787	7.880	-7.956	1.00	31.11	L111	C
ATOM	506	CD	PRO	A	74	-12.244	8.000	-7.601	1.00	35.28	L111	C
ATOM	507	N	ALA	A	75	-9.868	10.570	-4.348	1.00	31.58	L111	N
ATOM	508	CA	ALA	A	75	-9.763	11.862	-3.698	1.00	29.59	L111	C
ATOM	509	C	ALA	A	75	-9.517	12.901	-4.774	1.00	34.00	L111	C
ATOM	510	O	ALA	A	75	-10.210	13.915	-4.837	1.00	37.52	L111	O
ATOM	511	CB	ALA	A	75	-8.618	11.856	-2.694	1.00	34.28	L111	C
ATOM	512	N	SER	A	76	-8.532	12.638	-5.627	1.00	30.09	L111	N
ATOM	513	CA	SER	A	76	-8.211	13.561	-6.702	1.00	31.31	L111	C
ATOM	514	C	SER	A	76	-9.467	13.929	-7.483	1.00	31.25	L111	C
ATOM	515	O	SER	A	76	-9.661	15.091	-7.825	1.00	36.66	L111	O
ATOM	516	CB	SER	A	76	-7.169	12.951	-7.643	1.00	32.45	L111	C
ATOM	517	OG	SER	A	76	-7.473	11.608	-7.957	1.00	36.38	L111	O
ATOM	518	N	PHE	A	77	-10.323	12.946	-7.752	1.00	31.85	L111	N
ATOM	519	CA	PHE	A	77	-11.564	13.194	-8.489	1.00	34.16	L111	C
ATOM	520	C	PHE	A	77	-12.502	14.125	-7.734	1.00	38.37	L111	C
ATOM	521	O	PHE	A	77	-12.919	15.160	-8.251	1.00	41.67	L111	O
ATOM	522	CB	PHE	A	77	-12.307	11.894	-8.769	1.00	33.17	L111	C
ATOM	523	CG	PHE	A	77	-13.623	12.095	-9.468	1.00	40.76	L111	C
ATOM	524	CD1	PHE	A	77	-13.667	12.357	-10.837	1.00	47.11	L111	C
ATOM	525	CD2	PHE	A	77	-14.818	12.034	-8.761	1.00	42.42	L111	C
ATOM	526	CE1	PHE	A	77	-14.880	12.554	-11.492	1.00	38.82	L111	C
ATOM	527	CE2	PHE	A	77	-16.041	12.230	-9.409	1.00	42.68	L111	C
ATOM	528	CZ	PHE	A	77	-16.069	12.491	-10.777	1.00	38.85	L111	C
ATOM	529	N	LEU	A	78	-12.852	13.743	-6.514	1.00	39.27	L111	N
ATOM	530	CA	LEU	A	78	-13.732	14.568	-5.703	1.00	42.01	L111	C
ATOM	531	C	LEU	A	78	-13.162	15.986	-5.625	1.00	44.64	L111	C
ATOM	532	O	LEU	A	78	-13.892	16.967	-5.777	1.00	45.86	L111	O

ATOM	533	CB	LEU	A	78	-13.861	13.966	-4.303	1.00	42.80	L111	C
ATOM	534	CG	LEU	A	78	-14.640	12.646	-4.258	1.00	47.12	L111	C
ATOM	535	CD1	LEU	A	78	-14.485	11.973	-2.899	1.00	38.14	L111	C
ATOM	536	CD2	LEU	A	78	-16.108	12.925	-4.548	1.00	50.88	L111	C
ATOM	537	N	LEU	A	79	-11.851	16.081	-5.406	1.00	43.07	L111	N
ATOM	538	CA	LEU	A	79	-11.164	17.367	-5.309	1.00	34.91	L111	C
ATOM	539	C	LEU	A	79	-11.352	18.182	-6.580	1.00	35.68	L111	C
ATOM	540	O	LEU	A	79	-11.701	19.355	-6.522	1.00	36.29	L111	O
ATOM	541	CB	LEU	A	79	-9.676	17.150	-5.056	1.00	32.85	L111	C
ATOM	542	CG	LEU	A	79	-9.326	16.833	-3.603	1.00	29.72	L111	C
ATOM	543	CD1	LEU	A	79	-7.848	16.529	-3.480	1.00	33.33	L111	C
ATOM	544	CD2	LEU	A	79	-9.703	18.013	-2.730	1.00	29.46	L111	C
ATOM	545	N	LYS	A	80	-11.113	17.558	-7.727	1.00	39.06	L111	N
ATOM	546	CA	LYS	A	80	-11.292	18.235	-9.006	1.00	38.30	L111	C
ATOM	547	C	LYS	A	80	-12.692	18.832	-8.990	1.00	39.56	L111	C
ATOM	548	O	LYS	A	80	-12.872	20.036	-9.144	1.00	44.34	L111	O
ATOM	549	CB	LYS	A	80	-11.191	17.239	-10.163	1.00	32.02	L111	C
ATOM	550	CG	LYS	A	80	-9.805	17.066	-10.750	1.00	32.26	L111	C
ATOM	551	CD	LYS	A	80	-9.758	15.821	-11.628	1.00	37.75	L111	C
ATOM	552	CE	LYS	A	80	-8.410	15.660	-12.313	1.00	49.50	L111	C
ATOM	553	NZ	LYS	A	80	-8.046	14.224	-12.490	1.00	54.98	L111	N
ATOM	554	N	LYS	A	81	-13.681	17.969	-8.789	1.00	39.53	L111	N
ATOM	555	CA	LYS	A	81	-15.070	18.386	-8.754	1.00	38.23	L111	C
ATOM	556	C	LYS	A	81	-15.268	19.576	-7.832	1.00	41.10	L111	C
ATOM	557	O	LYS	A	81	-15.797	20.603	-8.242	1.00	50.63	L111	O
ATOM	558	CB	LYS	A	81	-15.949	17.230	-8.290	1.00	40.15	L111	C
ATOM	559	CG	LYS	A	81	-17.433	17.521	-8.367	1.00	56.64	L111	C
ATOM	560	CD	LYS	A	81	-18.209	16.317	-8.878	1.00	68.16	L111	C
ATOM	561	CE	LYS	A	81	-19.133	15.761	-7.799	1.00	76.64	L111	C
ATOM	562	NZ	LYS	A	81	-18.420	15.535	-6.502	1.00	78.09	L111	N
ATOM	563	N	ALA	A	82	-14.836	19.435	-6.585	1.00	45.28	L111	N
ATOM	564	CA	ALA	A	82	-14.976	20.500	-5.598	1.00	43.40	L111	C
ATOM	565	C	ALA	A	82	-14.384	21.832	-6.056	1.00	49.00	L111	C
ATOM	566	O	ALA	A	82	-15.003	22.884	-5.892	1.00	53.59	L111	O
ATOM	567	CB	ALA	A	82	-14.330	20.076	-4.290	1.00	42.16	L111	C
ATOM	568	N	ALA	A	83	-13.183	21.790	-6.621	1.00	48.31	L111	N
ATOM	569	CA	ALA	A	83	-12.527	23.004	-7.089	1.00	44.61	L111	C
ATOM	570	C	ALA	A	83	-13.115	23.458	-8.416	1.00	44.02	L111	C
ATOM	571	O	ALA	A	83	-12.693	24.467	-8.978	1.00	50.26	L111	O
ATOM	572	CB	ALA	A	83	-11.042	22.764	-7.236	1.00	40.08	L111	C
ATOM	573	N	GLY	A	84	-14.086	22.699	-8.912	1.00	42.49	L111	N
ATOM	574	CA	GLY	A	84	-14.727	23.029	-10.169	1.00	37.87	L111	C
ATOM	575	C	GLY	A	84	-13.804	22.971	-11.370	1.00	39.67	L111	C
ATOM	576	O	GLY	A	84	-14.127	23.511	-12.424	1.00	50.03	L111	O
ATOM	577	N	ILE	A	85	-12.654	22.323	-11.226	1.00	37.41	L111	N

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ATOM   578 CA  ILE A  85   -11.715  22.219 -12.334  1.00 37.65    L111 C
ATOM   579 C   ILE A  85   -11.826  20.868 -13.037  1.00 41.62    L111 C
ATOM   580 O   ILE A  85   -12.532  19.974 -12.571  1.00 45.50    L111 O
ATOM   581 CB  ILE A  85   -10.261  22.429 -11.863  1.00 37.93    L111 C
ATOM   582 CG1 ILE A  85    -9.905  21.408 -10.784  1.00 32.73    L111 C
ATOM   583 CG2 ILE A  85   -10.088  23.845 -11.336  1.00 42.04    L111 C
ATOM   584 CD1 ILE A  85    -8.435  21.395 -10.442  1.00 22.67    L111 C
ATOM   585 N   GLU A  86   -11.126  20.728 -14.159  1.00 45.67    L111 N
ATOM   586 CA  GLU A  86   -11.156  19.499 -14.948  1.00 47.13    L111 C
ATOM   587 C   GLU A  86    -9.874  18.675 -14.831  1.00 47.71    L111 C
ATOM   588 O   GLU A  86    -9.882  17.460 -15.044  1.00 48.51    L111 O
ATOM   589 CB  GLU A  86   -11.408  19.839 -16.421  1.00 57.79    L111 C
ATOM   590 CG  GLU A  86   -12.374  18.896 -17.128  1.00 77.13    L111 C
ATOM   591 CD  GLU A  86   -13.815  19.383 -17.078  1.00 86.58    L111 C
ATOM   592 OE1 GLU A  86   -14.025  20.594 -16.849  1.00 90.24    L111 O
ATOM   593 OE2 GLU A  86   -14.734  18.553 -17.268  1.00 89.81    L111 O
ATOM   594 N   LYS A  87    -8.771  19.335 -14.499  1.00 39.94    L111 N
ATOM   595 CA  LYS A  87    -7.499  18.645 -14.366  1.00 38.76    L111 C
ATOM   596 C   LYS A  87    -6.699  19.204 -13.204  1.00 34.61    L111 C
ATOM   597 O   LYS A  87    -6.981  20.291 -12.715  1.00 46.69    L111 O
ATOM   598 CB  LYS A  87    -6.686  18.784 -15.656  1.00 41.37    L111 C
ATOM   599 CG  LYS A  87    -7.279  18.057 -16.847  1.00 47.04    L111 C
ATOM   600 CD  LYS A  87    -6.550  18.426 -18.128  1.00 53.23    L111 C
ATOM   601 CE  LYS A  87    -5.833  17.224 -18.724  1.00 60.76    L111 C
ATOM   602 NZ  LYS A  87    -6.109  15.961 -17.979  1.00 61.63    L111 N
ATOM   603 N   GLY A  88    -5.703  18.452 -12.759  1.00 34.29    L111 N
ATOM   604 CA  GLY A  88    -4.871  18.914 -11.669  1.00 33.53    L111 C
ATOM   605 C   GLY A  88    -3.718  19.688 -12.261  1.00 35.94    L111 C
ATOM   606 O   GLY A  88    -3.422  19.547 -13.445  1.00 37.03    L111 O
ATOM   607 N   SER A  89    -3.065  20.511 -11.453  1.00 35.86    L111 N
ATOM   608 CA  SER A  89    -1.941  21.285 -11.951  1.00 31.79    L111 C
ATOM   609 C   SER A  89    -0.968  20.358 -12.658  1.00 33.45    L111 C
ATOM   610 O   SER A  89    -0.868  19.185 -12.317  1.00 36.12    L111 O
ATOM   611 CB  SER A  89    -1.227  21.987 -10.801  1.00 30.17    L111 C
ATOM   612 OG  SER A  89     0.141  22.195 -11.114  1.00 29.65    L111 O
ATOM   613 N   SER A  90    -0.260  20.881 -13.651  1.00 36.82    L111 N
ATOM   614 CA  SER A  90     0.716  20.083 -14.372  1.00 35.62    L111 C
ATOM   615 C   SER A  90     1.981  20.112 -13.530  1.00 35.74    L111 C
ATOM   616 O   SER A  90     2.879  19.287 -13.692  1.00 37.58    L111 O
ATOM   617 CB  SER A  90     0.976  20.682 -15.758  1.00 37.33    L111 C
ATOM   618 OG  SER A  90     1.955  21.708 -15.701  1.00 51.94    L111 O
ATOM   619 N   GLU A  91     2.034  21.083 -12.625  1.00 33.32    L111 N
ATOM   620 CA  GLU A  91     3.166  21.246 -11.726  1.00 38.55    L111 C
ATOM   621 C   GLU A  91     2.619  21.648 -10.362  1.00 37.86    L111 C
ATOM   622 O   GLU A  91     2.553  22.832 -10.026  1.00 36.53    L111 O
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ATOM  623  CB  GLU A  91      4.115  22.317 -12.262  1.00 42.92      L111 C
ATOM  624  CG  GLU A  91      4.927  21.857 -13.457  1.00 56.44      L111 C
ATOM  625  CD  GLU A  91      6.025  22.832 -13.841  1.00 69.04      L111 C
ATOM  626  OE1 GLU A  91      6.223  23.832 -13.113  1.00 67.53      L111 O
ATOM  627  OE2 GLU A  91      6.692  22.593 -14.876  1.00 73.04      L111 O
ATOM  628  N   PRO A  92      2.199  20.652  -9.561  1.00 39.75      L111 N
ATOM  629  CA  PRO A  92      1.643  20.871  -8.222  1.00 37.71      L111 C
ATOM  630  C   PRO A  92      2.536  21.749  -7.365  1.00 33.98      L111 C
ATOM  631  O   PRO A  92      3.760  21.633  -7.418  1.00 31.75      L111 O
ATOM  632  CB  PRO A  92      1.505  19.459  -7.655  1.00 34.90      L111 C
ATOM  633  CG  PRO A  92      1.371  18.596  -8.852  1.00 30.25      L111 C
ATOM  634  CD  PRO A  92      2.246  19.219  -9.898  1.00 39.42      L111 C
ATOM  635  N   LYS A  93      1.910  22.625  -6.584  1.00 30.90      L111 N
ATOM  636  CA  LYS A  93      2.620  23.544  -5.703  1.00 36.65      L111 C
ATOM  637  C   LYS A  93      3.250  24.695  -6.477  1.00 36.64      L111 C
ATOM  638  O   LYS A  93      3.181  25.841  -6.044  1.00 45.57      L111 O
ATOM  639  CB  LYS A  93      3.699  22.800  -4.907  1.00 42.76      L111 C
ATOM  640  CG  LYS A  93      4.532  23.681  -3.993  1.00 47.27      L111 C
ATOM  641  CD  LYS A  93      4.991  22.907  -2.768  1.00 53.52      L111 C
ATOM  642  CE  LYS A  93      5.915  23.744  -1.894  1.00 54.40      L111 C
ATOM  643  NZ  LYS A  93      7.235  23.085  -1.673  1.00 61.73      L111 N
ATOM  644  N   ARG A  94      3.864  24.394  -7.616  1.00 35.63      L111 N
ATOM  645  CA  ARG A  94      4.486  25.432  -8.430  1.00 29.80      L111 C
ATOM  646  C   ARG A  94      3.408  26.252  -9.125  1.00 32.19      L111 C
ATOM  647  O   ARG A  94      3.593  27.443  -9.371  1.00 36.21      L111 O
ATOM  648  CB  ARG A  94      5.418  24.817  -9.475  1.00 21.41      L111 C
ATOM  649  CG  ARG A  94      6.818  24.559  -8.966  1.00 26.71      L111 C
ATOM  650  CD  ARG A  94      7.779  24.180 -10.088  1.00 28.16      L111 C
ATOM  651  NE  ARG A  94      9.002  23.582  -9.551  1.00 40.63      L111 N
ATOM  652  CZ  ARG A  94     10.016  23.133 -10.289  1.00 42.98      L111 C
ATOM  653  NH1 ARG A  94      9.965  23.212 -11.610  1.00 45.19      L111 N
ATOM  654  NH2 ARG A  94     11.085  22.606  -9.704  1.00 48.46      L111 N
ATOM  655  N   LYS A  95      2.284  25.612  -9.440  1.00 28.46      L111 N
ATOM  656  CA  LYS A  95      1.177  26.298 -10.104  1.00 30.94      L111 C
ATOM  657  C   LYS A  95     -0.145  25.834  -9.542  1.00 28.39      L111 C
ATOM  658  O   LYS A  95     -0.511  24.679  -9.700  1.00 40.28      L111 O
ATOM  659  CB  LYS A  95      1.169  26.024 -11.614  1.00 36.77      L111 C
ATOM  660  CG  LYS A  95      2.531  25.791 -12.244  1.00 49.47      L111 C
ATOM  661  CD  LYS A  95      2.426  25.746 -13.765  1.00 48.94      L111 C
ATOM  662  CE  LYS A  95      3.782  25.970 -14.420  1.00 50.63      L111 C
ATOM  663  NZ  LYS A  95      3.730  25.733 -15.886  1.00 46.96      L111 N
ATOM  664  N   ILE A  96     -0.872  26.728  -8.892  1.00 30.02      L111 N
ATOM  665  CA  ILE A  96     -2.162  26.357  -8.337  1.00 31.34      L111 C
ATOM  666  C   ILE A  96     -3.209  26.537  -9.425  1.00 35.19      L111 C
ATOM  667  O   ILE A  96     -3.286  27.593 -10.048  1.00 42.96      L111 O
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ATOM   668  CB  ILE A  96     -2.502  27.231  -7.115  1.00 33.87      L111 C
ATOM   669  CG1 ILE A  96     -1.379  27.115  -6.079  1.00 33.04      L111 C
ATOM   670  CG2 ILE A  96     -3.840  26.812  -6.518  1.00 28.64      L111 C
ATOM   671  CD1 ILE A  96     -0.892  25.695  -5.843  1.00 35.36      L111 C
ATOM   672  N   VAL A  97     -4.008  25.504  -9.664  1.00 32.56      L111 N
ATOM   673  CA  VAL A  97     -5.022  25.570 -10.704  1.00 29.74      L111 C
ATOM   674  C   VAL A  97     -6.427  25.650 -10.148  1.00 36.58      L111 C
ATOM   675  O   VAL A  97     -7.399  25.737 -10.905  1.00 38.60      L111 O
ATOM   676  CB  VAL A  97     -4.930  24.351 -11.648  1.00 38.47      L111 C
ATOM   677  CG1 VAL A  97     -3.502  24.185 -12.123  1.00 37.01      L111 C
ATOM   678  CG2 VAL A  97     -5.403  23.086 -10.940  1.00 37.97      L111 C
ATOM   679  N   GLY A  98     -6.531  25.623  -8.823  1.00 35.02      L111 N
ATOM   680  CA  GLY A  98     -7.836  25.690  -8.192  1.00 35.16      L111 C
ATOM   681  C   GLY A  98     -7.744  25.779  -6.683  1.00 38.01      L111 C
ATOM   682  O   GLY A  98     -6.648  25.832  -6.117  1.00 38.34      L111 O
ATOM   683  N   LYS A  99     -8.896  25.801  -6.023  1.00 35.14      L111 N
ATOM   684  CA  LYS A  99     -8.911  25.883  -4.575  1.00 40.57      L111 C
ATOM   685  C   LYS A  99    -10.230  25.403  -3.991  1.00 42.95      L111 C
ATOM   686  O   LYS A  99    -11.264  25.396  -4.663  1.00 42.23      L111 O
ATOM   687  CB  LYS A  99     -8.634  27.320  -4.130  1.00 50.99      L111 C
ATOM   688  CG  LYS A  99     -9.850  28.231  -4.172  1.00 60.57      L111 C
ATOM   689  CD  LYS A  99     -9.469  29.678  -3.885  1.00 65.97      L111 C
ATOM   690  CE  LYS A  99    -10.646  30.614  -4.127  1.00 63.49      L111 C
ATOM   691  NZ  LYS A  99    -10.216  31.886  -4.768  1.00 65.04      L111 N
ATOM   692  N   VAL A 100    -10.180  24.992  -2.731  1.00 40.70      L111 N
ATOM   693  CA  VAL A 100    -11.361  24.511  -2.036  1.00 41.33      L111 C
ATOM   694  C   VAL A 100    -11.330  24.980  -0.592  1.00 41.84      L111 C
ATOM   695  O   VAL A 100    -10.263  25.188  -0.012  1.00 40.91      L111 O
ATOM   696  CB  VAL A 100    -11.440  22.973  -2.057  1.00 42.37      L111 C
ATOM   697  CG1 VAL A 100    -11.840  22.498  -3.442  1.00 43.81      L111 C
ATOM   698  CG2 VAL A 100    -10.102  22.377  -1.651  1.00 37.38      L111 C
ATOM   699  N   THR A 101    -12.511  25.145  -0.016  1.00 43.68      L111 N
ATOM   700  CA  THR A 101    -12.629  25.595   1.355  1.00 42.43      L111 C
ATOM   701  C   THR A 101    -12.362  24.454   2.321  1.00 45.89      L111 C
ATOM   702  O   THR A 101    -12.495  23.284   1.963  1.00 46.60      L111 O
ATOM   703  CB  THR A 101    -14.026  26.153   1.610  1.00 45.72      L111 C
ATOM   704  OG1 THR A 101    -15.005  25.154   1.293  1.00 40.56      L111 O
ATOM   705  CG2 THR A 101    -14.260  27.380   0.738  1.00 42.52      L111 C
ATOM   706  N   ARG A 102    -11.981  24.799   3.545  1.00 49.33      L111 N
ATOM   707  CA  ARG A 102    -11.701  23.797   4.565  1.00 49.44      L111 C
ATOM   708  C   ARG A 102    -12.925  22.925   4.792  1.00 49.34      L111 C
ATOM   709  O   ARG A 102    -12.807  21.744   5.115  1.00 53.45      L111 O
ATOM   710  CB  ARG A 102    -11.301  24.469   5.879  1.00 51.60      L111 C
ATOM   711  CG  ARG A 102    -10.126  23.806   6.574  1.00 64.32      L111 C
ATOM   712  CD  ARG A 102    -10.579  23.003   7.777  1.00 72.71      L111 C
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ATOM	713	NE	ARG	A	102	-10.495	23.786	9.006	1.00	86.85	L111	N
ATOM	714	CZ	ARG	A	102	-10.080	23.304	10.174	1.00	96.04	L111	C
ATOM	715	NH1	ARG	A	102	-9.710	22.033	10.275	1.00	95.91	L111	N
ATOM	716	NH2	ARG	A	102	-10.033	24.095	11.242	1.00	96.71	L111	N
ATOM	717	N	LYS	A	103	-14.103	23.514	4.626	1.00	50.48	L111	N
ATOM	718	CA	LYS	A	103	-15.341	22.774	4.811	1.00	51.76	L111	C
ATOM	719	C	LYS	A	103	-15.441	21.718	3.719	1.00	51.34	L111	C
ATOM	720	O	LYS	A	103	-15.884	20.600	3.966	1.00	59.36	L111	O
ATOM	721	CB	LYS	A	103	-16.545	23.721	4.751	1.00	53.67	L111	C
ATOM	722	CG	LYS	A	103	-17.839	23.135	5.319	1.00	62.90	L111	C
ATOM	723	CD	LYS	A	103	-17.717	22.781	6.806	1.00	65.48	L111	C
ATOM	724	CE	LYS	A	103	-18.840	21.841	7.257	1.00	63.76	L111	C
ATOM	725	NZ	LYS	A	103	-19.077	21.884	8.732	1.00	58.26	L111	N
ATOM	726	N	GLN	A	104	-15.013	22.073	2.512	1.00	51.89	L111	N
ATOM	727	CA	GLN	A	104	-15.052	21.145	1.388	1.00	44.08	L111	C
ATOM	728	C	GLN	A	104	-14.161	19.939	1.664	1.00	42.43	L111	C
ATOM	729	O	GLN	A	104	-14.519	18.804	1.347	1.00	40.53	L111	O
ATOM	730	CB	GLN	A	104	-14.602	21.850	0.110	1.00	42.64	L111	C
ATOM	731	CG	GLN	A	104	-15.663	22.751	-0.484	1.00	35.82	L111	C
ATOM	732	CD	GLN	A	104	-15.242	23.354	-1.804	1.00	44.67	L111	C
ATOM	733	OE1	GLN	A	104	-14.303	24.154	-1.867	1.00	37.53	L111	O
ATOM	734	NE2	GLN	A	104	-15.936	22.975	-2.873	1.00	35.39	L111	N
ATOM	735	N	ILE	A	105	-12.998	20.186	2.254	1.00	39.32	L111	N
ATOM	736	CA	ILE	A	105	-12.088	19.103	2.584	1.00	35.57	L111	C
ATOM	737	C	ILE	A	105	-12.846	18.187	3.525	1.00	41.32	L111	C
ATOM	738	O	ILE	A	105	-12.770	16.965	3.411	1.00	46.00	L111	O
ATOM	739	CB	ILE	A	105	-10.832	19.624	3.298	1.00	33.68	L111	C
ATOM	740	CG1	ILE	A	105	-9.873	20.242	2.277	1.00	32.96	L111	C
ATOM	741	CG2	ILE	A	105	-10.154	18.495	4.061	1.00	34.33	L111	C
ATOM	742	CD1	ILE	A	105	-9.501	19.321	1.131	1.00	34.42	L111	C
ATOM	743	N	GLU	A	106	-13.584	18.800	4.448	1.00	47.08	L111	N
ATOM	744	CA	GLU	A	106	-14.382	18.068	5.428	1.00	53.52	L111	C
ATOM	745	C	GLU	A	106	-15.411	17.186	4.719	1.00	55.13	L111	C
ATOM	746	O	GLU	A	106	-15.606	16.027	5.087	1.00	59.36	L111	O
ATOM	747	CB	GLU	A	106	-15.094	19.051	6.381	1.00	50.72	L111	C
ATOM	748	CG	GLU	A	106	-15.480	18.464	7.748	1.00	55.56	L111	C
ATOM	749	CD	GLU	A	106	-16.029	19.504	8.734	1.00	62.03	L111	C
ATOM	750	OE1	GLU	A	106	-15.308	20.476	9.054	1.00	63.26	L111	O
ATOM	751	OE2	GLU	A	106	-17.182	19.345	9.199	1.00	53.90	L111	O
ATOM	752	N	GLU	A	107	-16.061	17.731	3.695	1.00	51.75	L111	N
ATOM	753	CA	GLU	A	107	-17.071	16.982	2.954	1.00	52.07	L111	C
ATOM	754	C	GLU	A	107	-16.476	15.755	2.282	1.00	50.13	L111	C
ATOM	755	O	GLU	A	107	-16.990	14.642	2.417	1.00	49.53	L111	O
ATOM	756	CB	GLU	A	107	-17.720	17.871	1.891	1.00	56.84	L111	C
ATOM	757	CG	GLU	A	107	-17.859	19.328	2.293	1.00	73.20	L111	C

ATOM	758	CD	GLU	A	107	-18.843	20.088	1.422	1.00	81.27	L111	C
ATOM	759	OE1	GLU	A	107	-19.271	19.540	0.382	1.00	84.05	L111	O
ATOM	760	OE2	GLU	A	107	-19.187	21.237	1.779	1.00	86.15	L111	O
ATOM	761	N	ILE	A	108	-15.391	15.973	1.549	1.00	46.89	L111	N
ATOM	762	CA	ILE	A	108	-14.719	14.900	0.844	1.00	39.41	L111	C
ATOM	763	C	ILE	A	108	-14.222	13.854	1.829	1.00	40.77	L111	C
ATOM	764	O	ILE	A	108	-14.441	12.658	1.637	1.00	43.65	L111	O
ATOM	765	CB	ILE	A	108	-13.542	15.447	0.019	1.00	38.05	L111	C
ATOM	766	CG1	ILE	A	108	-14.072	16.428	-1.032	1.00	36.44	L111	C
ATOM	767	CG2	ILE	A	108	-12.796	14.305	-0.649	1.00	41.19	L111	C
ATOM	768	CD1	ILE	A	108	-13.004	17.084	-1.882	1.00	31.78	L111	C
ATOM	769	N	ALA	A	109	-13.561	14.303	2.891	1.00	40.57	L111	N
ATOM	770	CA	ALA	A	109	-13.053	13.380	3.895	1.00	42.41	L111	C
ATOM	771	C	ALA	A	109	-14.205	12.546	4.429	1.00	44.77	L111	C
ATOM	772	O	ALA	A	109	-14.051	11.356	4.685	1.00	48.40	L111	O
ATOM	773	CB	ALA	A	109	-12.393	14.140	5.032	1.00	38.72	L111	C
ATOM	774	N	LYS	A	110	-15.365	13.174	4.589	1.00	47.97	L111	N
ATOM	775	CA	LYS	A	110	-16.537	12.474	5.099	1.00	44.59	L111	C
ATOM	776	C	LYS	A	110	-17.027	11.474	4.066	1.00	45.30	L111	C
ATOM	777	O	LYS	A	110	-17.377	10.342	4.401	1.00	44.67	L111	O
ATOM	778	CB	LYS	A	110	-17.651	13.469	5.422	1.00	45.45	L111	C
ATOM	779	CG	LYS	A	110	-17.991	13.562	6.902	1.00	47.29	L111	C
ATOM	780	CD	LYS	A	110	-17.733	14.963	7.448	1.00	51.84	L111	C
ATOM	781	CE	LYS	A	110	-18.991	15.558	8.070	1.00	53.58	L111	C
ATOM	782	NZ	LYS	A	110	-18.712	16.257	9.356	1.00	55.16	L111	N
ATOM	783	N	THR	A	111	-17.043	11.902	2.807	1.00	44.49	L111	N
ATOM	784	CA	THR	A	111	-17.492	11.060	1.705	1.00	42.63	L111	C
ATOM	785	C	THR	A	111	-16.635	9.810	1.548	1.00	44.42	L111	C
ATOM	786	O	THR	A	111	-17.149	8.707	1.375	1.00	44.77	L111	O
ATOM	787	CB	THR	A	111	-17.452	11.830	0.376	1.00	40.13	L111	C
ATOM	788	OG1	THR	A	111	-18.545	12.754	0.325	1.00	46.15	L111	O
ATOM	789	CG2	THR	A	111	-17.552	10.871	-0.799	1.00	43.65	L111	C
ATOM	790	N	LYS	A	112	-15.323	9.995	1.609	1.00	42.25	L111	N
ATOM	791	CA	LYS	A	112	-14.382	8.898	1.448	1.00	42.77	L111	C
ATOM	792	C	LYS	A	112	-14.081	8.127	2.732	1.00	43.93	L111	C
ATOM	793	O	LYS	A	112	-13.321	7.157	2.713	1.00	47.28	L111	O
ATOM	794	CB	LYS	A	112	-13.072	9.442	0.873	1.00	44.33	L111	C
ATOM	795	CG	LYS	A	112	-13.129	9.772	-0.607	1.00	40.93	L111	C
ATOM	796	CD	LYS	A	112	-11.806	9.474	-1.281	1.00	35.66	L111	C
ATOM	797	CE	LYS	A	112	-11.377	8.032	-1.062	1.00	31.03	L111	C
ATOM	798	NZ	LYS	A	112	-11.960	7.113	-2.076	1.00	28.57	L111	N
ATOM	799	N	MET	A	113	-14.673	8.554	3.842	1.00	42.32	L111	N
ATOM	800	CA	MET	A	113	-14.436	7.911	5.132	1.00	41.26	L111	C
ATOM	801	C	MET	A	113	-14.492	6.379	5.116	1.00	39.35	L111	C
ATOM	802	O	MET	A	113	-13.619	5.717	5.688	1.00	39.20	L111	O

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ATOM  803  CB  MET A 113    -15.410   8.457   6.177  1.00 39.84      L111 C
ATOM  804  CG  MET A 113    -14.931   8.283   7.609  1.00 45.81      L111 C
ATOM  805  SD  MET A 113    -13.481   9.269   8.040  1.00 47.31      L111 S
ATOM  806  CE  MET A 113    -14.261  10.787   8.610  1.00 49.60      L111 C
ATOM  807  N   PRO A 114    -15.524   5.793   4.484  1.00 32.93      L111 N
ATOM  808  CA  PRO A 114    -15.582   4.328   4.458  1.00 29.51      L111 C
ATOM  809  C   PRO A 114    -14.301   3.703   3.912  1.00 35.05      L111 C
ATOM  810  O   PRO A 114    -13.918   2.609   4.314  1.00 41.74      L111 O
ATOM  811  CB  PRO A 114    -16.791   4.013   3.575  1.00 27.80      L111 C
ATOM  812  CG  PRO A 114    -17.214   5.307   2.967  1.00 23.57      L111 C
ATOM  813  CD  PRO A 114    -16.678   6.411   3.811  1.00 31.92      L111 C
ATOM  814  N   ASP A 115    -13.629   4.408   3.008  1.00 38.82      L111 N
ATOM  815  CA  ASP A 115    -12.399   3.898   2.419  1.00 36.41      L111 C
ATOM  816  C   ASP A 115    -11.138   4.462   3.069  1.00 36.55      L111 C
ATOM  817  O   ASP A 115    -10.025   4.080   2.713  1.00 40.35      L111 O
ATOM  818  CB  ASP A 115    -12.385   4.193   0.919  1.00 48.68      L111 C
ATOM  819  CG  ASP A 115    -13.453   3.418   0.162  1.00 57.41      L111 C
ATOM  820  OD1 ASP A 115    -13.653   2.221   0.464  1.00 51.55      L111 O
ATOM  821  OD2 ASP A 115    -14.090   4.009  -0.737  1.00 58.21      L111 O
ATOM  822  N   LEU A 116    -11.311   5.368   4.024  1.00 38.89      L111 N
ATOM  823  CA  LEU A 116    -10.178   5.969   4.720  1.00 33.57      L111 C
ATOM  824  C   LEU A 116     -9.916   5.199   6.007  1.00 32.97      L111 C
ATOM  825  O   LEU A 116    -10.817   4.567   6.547  1.00 40.69      L111 O
ATOM  826  CB  LEU A 116    -10.482   7.427   5.055  1.00 38.53      L111 C
ATOM  827  CG  LEU A 116     -9.930   8.533   4.156  1.00 37.13      L111 C
ATOM  828  CD1 LEU A 116     -9.839   8.062   2.720  1.00 34.98      L111 C
ATOM  829  CD2 LEU A 116    -10.837   9.742   4.261  1.00 33.33      L111 C
ATOM  830  N   ASN A 117     -8.686   5.256   6.501  1.00 32.67      L111 N
ATOM  831  CA  ASN A 117     -8.336   4.549   7.725  1.00 33.28      L111 C
ATOM  832  C   ASN A 117     -8.052   5.502   8.889  1.00 39.76      L111 C
ATOM  833  O   ASN A 117     -7.373   5.140   9.851  1.00 36.63      L111 O
ATOM  834  CB  ASN A 117     -7.117   3.666   7.475  1.00 23.35      L111 C
ATOM  835  CG  ASN A 117     -5.872   4.470   7.208  1.00 24.02      L111 C
ATOM  836  OD1 ASN A 117     -5.949   5.659   6.916  1.00 31.18      L111 O
ATOM  837  ND2 ASN A 117     -4.714   3.828   7.306  1.00 18.87      L111 N
ATOM  838  N   ALA A 118     -8.572   6.720   8.799  1.00 41.20      L111 N
ATOM  839  CA  ALA A 118     -8.363   7.710   9.846  1.00 41.18      L111 C
ATOM  840  C   ALA A 118     -9.297   7.443  11.018  1.00 43.82      L111 C
ATOM  841  O   ALA A 118    -10.455   7.069  10.827  1.00 45.81      L111 O
ATOM  842  CB  ALA A 118     -8.604   9.103   9.296  1.00 41.30      L111 C
ATOM  843  N   ASN A 119     -8.793   7.644  12.230  1.00 42.07      L111 N
ATOM  844  CA  ASN A 119     -9.589   7.419  13.429  1.00 42.41      L111 C
ATOM  845  C   ASN A 119    -10.370   8.660  13.847  1.00 48.14      L111 C
ATOM  846  O   ASN A 119    -11.141   8.625  14.807  1.00 53.14      L111 O
ATOM  847  CB  ASN A 119     -8.684   6.981  14.575  1.00 37.27      L111 C
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ATOM	848	CG	ASN	A	119	-8.180	5.575	14.400	1.00	33.45	L111	C
ATOM	849	OD1	ASN	A	119	-8.886	4.714	13.876	1.00	31.47	L111	O
ATOM	850	ND2	ASN	A	119	-6.951	5.328	14.837	1.00	38.73	L111	N
ATOM	851	N	SER	A	120	-10.168	9.756	13.125	1.00	48.44	L111	N
ATOM	852	CA	SER	A	120	-10.851	11.005	13.430	1.00	43.86	L111	C
ATOM	853	C	SER	A	120	-11.091	11.809	12.163	1.00	45.90	L111	C
ATOM	854	O	SER	A	120	-10.321	11.715	11.208	1.00	53.71	L111	O
ATOM	855	CB	SER	A	120	-10.010	11.834	14.401	1.00	38.80	L111	C
ATOM	856	OG	SER	A	120	-8.642	11.834	14.030	1.00	32.06	L111	O
ATOM	857	N	LEU	A	121	-12.157	12.601	12.156	1.00	46.97	L111	N
ATOM	858	CA	LEU	A	121	-12.476	13.429	11.000	1.00	44.83	L111	C
ATOM	859	C	LEU	A	121	-11.297	14.333	10.678	1.00	45.31	L111	C
ATOM	860	O	LEU	A	121	-11.078	14.693	9.526	1.00	52.25	L111	O
ATOM	861	CB	LEU	A	121	-13.705	14.291	11.277	1.00	39.77	L111	C
ATOM	862	CG	LEU	A	121	-13.904	15.469	10.325	1.00	41.18	L111	C
ATOM	863	CD1	LEU	A	121	-14.063	14.958	8.900	1.00	41.06	L111	C
ATOM	864	CD2	LEU	A	121	-15.128	16.260	10.751	1.00	41.00	L111	C
ATOM	865	N	GLU	A	122	-10.542	14.701	11.705	1.00	46.54	L111	N
ATOM	866	CA	GLU	A	122	-9.383	15.562	11.522	1.00	47.46	L111	C
ATOM	867	C	GLU	A	122	-8.327	14.834	10.702	1.00	45.12	L111	C
ATOM	868	O	GLU	A	122	-7.781	15.383	9.747	1.00	51.65	L111	O
ATOM	869	CB	GLU	A	122	-8.807	15.962	12.881	1.00	45.32	L111	C
ATOM	870	CG	GLU	A	122	-9.646	16.987	13.629	1.00	57.78	L111	C
ATOM	871	CD	GLU	A	122	-10.643	16.353	14.588	1.00	63.03	L111	C
ATOM	872	OE1	GLU	A	122	-10.380	15.234	15.075	1.00	64.43	L111	O
ATOM	873	OE2	GLU	A	122	-11.690	16.979	14.857	1.00	69.35	L111	O
ATOM	874	N	ALA	A	123	-8.045	13.593	11.083	1.00	41.17	L111	N
ATOM	875	CA	ALA	A	123	-7.062	12.786	10.381	1.00	38.97	L111	C
ATOM	876	C	ALA	A	123	-7.516	12.566	8.944	1.00	41.17	L111	C
ATOM	877	O	ALA	A	123	-6.701	12.562	8.022	1.00	41.16	L111	O
ATOM	878	CB	ALA	A	123	-6.891	11.452	11.081	1.00	36.50	L111	C
ATOM	879	N	ALA	A	124	-8.822	12.389	8.760	1.00	36.64	L111	N
ATOM	880	CA	ALA	A	124	-9.390	12.168	7.432	1.00	36.26	L111	C
ATOM	881	C	ALA	A	124	-9.133	13.362	6.533	1.00	35.14	L111	C
ATOM	882	O	ALA	A	124	-8.742	13.207	5.379	1.00	41.09	L111	O
ATOM	883	CB	ALA	A	124	-10.886	11.914	7.533	1.00	32.82	L111	C
ATOM	884	N	MET	A	125	-9.358	14.555	7.072	1.00	38.73	L111	N
ATOM	885	CA	MET	A	125	-9.158	15.785	6.322	1.00	34.84	L111	C
ATOM	886	C	MET	A	125	-7.686	15.968	6.003	1.00	31.87	L111	C
ATOM	887	O	MET	A	125	-7.330	16.458	4.938	1.00	42.09	L111	O
ATOM	888	CB	MET	A	125	-9.671	16.977	7.126	1.00	35.51	L111	C
ATOM	889	CG	MET	A	125	-11.072	16.769	7.695	1.00	40.88	L111	C
ATOM	890	SD	MET	A	125	-12.008	18.287	7.948	1.00	45.99	L111	S
ATOM	891	CE	MET	A	125	-10.675	19.462	8.286	1.00	44.96	L111	C
ATOM	892	N	LYS	A	126	-6.831	15.567	6.930	1.00	28.09	L111	N

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ATOM   893  CA  LYS A 126     -5.397  15.684   6.730  1.00 28.15      L111 C
ATOM   894  C   LYS A 126     -5.007  14.801   5.551  1.00 30.29      L111 C
ATOM   895  O   LYS A 126     -4.107  15.129   4.781  1.00 32.85      L111 O
ATOM   896  CB  LYS A 126     -4.652  15.229   7.989  1.00 34.95      L111 C
ATOM   897  CG  LYS A 126     -4.010  16.351   8.781  1.00 28.05      L111 C
ATOM   898  CD  LYS A 126     -4.465  16.328  10.229  1.00 31.31      L111 C
ATOM   899  CE  LYS A 126     -3.431  15.676  11.140  1.00 39.80      L111 C
ATOM   900  NZ  LYS A 126     -2.064  16.271  11.016  1.00 45.29      L111 N
ATOM   901  N   ILE A 127     -5.691  13.669   5.417  1.00 32.92      L111 N
ATOM   902  CA  ILE A 127     -5.414  12.748   4.325  1.00 29.89      L111 C
ATOM   903  C   ILE A 127     -5.820  13.405   3.014  1.00 30.60      L111 C
ATOM   904  O   ILE A 127     -5.024  13.492   2.086  1.00 36.08      L111 O
ATOM   905  CB  ILE A 127     -6.179  11.423   4.501  1.00 23.98      L111 C
ATOM   906  CG1 ILE A 127     -5.591  10.649   5.689  1.00 33.32      L111 C
ATOM   907  CG2 ILE A 127     -6.074  10.590   3.234  1.00 26.83      L111 C
ATOM   908  CD1 ILE A 127     -6.427   9.465   6.152  1.00 25.44      L111 C
ATOM   909  N   ILE A 128     -7.060  13.875   2.947  1.00 30.31      L111 N
ATOM   910  CA  ILE A 128     -7.559  14.543   1.756  1.00 27.70      L111 C
ATOM   911  C   ILE A 128     -6.681  15.730   1.359  1.00 30.19      L111 C
ATOM   912  O   ILE A 128     -6.406  15.939   0.181  1.00 37.83      L111 O
ATOM   913  CB  ILE A 128     -8.980  15.065   1.974  1.00 29.26      L111 C
ATOM   914  CG1 ILE A 128     -9.911  13.906   2.325  1.00 27.20      L111 C
ATOM   915  CG2 ILE A 128     -9.454  15.802   0.731  1.00 29.10      L111 C
ATOM   916  CD1 ILE A 128     -9.915  12.793   1.304  1.00 21.41      L111 C
ATOM   917  N   GLU A 129     -6.245  16.507   2.342  1.00 27.35      L111 N
ATOM   918  CA  GLU A 129     -5.412  17.669   2.065  1.00 28.43      L111 C
ATOM   919  C   GLU A 129     -4.116  17.249   1.418  1.00 25.38      L111 C
ATOM   920  O   GLU A 129     -3.554  17.983   0.613  1.00 33.17      L111 O
ATOM   921  CB  GLU A 129     -5.092  18.429   3.348  1.00 39.34      L111 C
ATOM   922  CG  GLU A 129     -6.223  19.289   3.870  1.00 49.18      L111 C
ATOM   923  CD  GLU A 129     -6.093  19.546   5.355  1.00 57.36      L111 C
ATOM   924  OE1 GLU A 129     -4.942  19.571   5.849  1.00 62.27      L111 O
ATOM   925  OE2 GLU A 129     -7.136  19.716   6.024  1.00 61.09      L111 O
ATOM   926  N   GLY A 130     -3.634  16.071   1.785  1.00 24.18      L111 N
ATOM   927  CA  GLY A 130     -2.394  15.591   1.210  1.00 21.91      L111 C
ATOM   928  C   GLY A 130     -2.536  15.392  -0.285  1.00 23.19      L111 C
ATOM   929  O   GLY A 130     -1.597  15.625  -1.042  1.00 21.99      L111 O
ATOM   930  N   THR A 131     -3.720  14.962  -0.705  1.00 22.49      L111 N
ATOM   931  CA  THR A 131     -4.005  14.723  -2.111  1.00 25.94      L111 C
ATOM   932  C   THR A 131     -4.160  16.049  -2.849  1.00 28.86      L111 C
ATOM   933  O   THR A 131     -3.629  16.229  -3.946  1.00 31.66      L111 O
ATOM   934  CB  THR A 131     -5.292  13.896  -2.270  1.00 27.10      L111 C
ATOM   935  OG1 THR A 131     -5.078  12.577  -1.747  1.00 26.23      L111 O
ATOM   936  CG2 THR A 131     -5.694  13.808  -3.734  1.00 27.07      L111 C
ATOM   937  N   ALA A 132     -4.887  16.979  -2.241  1.00 27.56      L111 N
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ATOM    938  CA  ALA A 132      -5.096  18.292  -2.835  1.00 26.64      L111 C
ATOM    939  C   ALA A 132      -3.753  18.974  -3.058  1.00 28.30      L111 C
ATOM    940  O   ALA A 132      -3.524  19.602  -4.084  1.00 30.29      L111 O
ATOM    941  CB  ALA A 132      -5.954  19.134  -1.922  1.00 32.54      L111 C
ATOM    942  N   LYS A 133      -2.866  18.843  -2.082  1.00 29.52      L111 N
ATOM    943  CA  LYS A 133      -1.545  19.443  -2.158  1.00 27.21      L111 C
ATOM    944  C   LYS A 133      -0.754  18.848  -3.311  1.00 30.72      L111 C
ATOM    945  O   LYS A 133       0.190  19.458  -3.813  1.00 34.77      L111 O
ATOM    946  CB  LYS A 133      -0.784  19.205  -0.846  1.00 30.61      L111 C
ATOM    947  CG  LYS A 133      -0.843  20.371   0.138  1.00 38.23      L111 C
ATOM    948  CD  LYS A 133      -0.782  19.897   1.581  1.00 35.27      L111 C
ATOM    949  CE  LYS A 133       0.653  19.826   2.079  1.00 45.39      L111 C
ATOM    950  NZ  LYS A 133       0.737  19.680   3.568  1.00 50.50      L111 N
ATOM    951  N   SER A 134      -1.141  17.650  -3.729  1.00 31.51      L111 N
ATOM    952  CA  SER A 134      -0.441  16.966  -4.807  1.00 33.04      L111 C
ATOM    953  C   SER A 134      -0.969  17.300  -6.202  1.00 30.13      L111 C
ATOM    954  O   SER A 134      -0.345  16.952  -7.198  1.00 27.50      L111 O
ATOM    955  CB  SER A 134      -0.510  15.452  -4.588  1.00 31.88      L111 C
ATOM    956  OG  SER A 134      -1.741  14.927  -5.055  1.00 23.70      L111 O
ATOM    957  N   MET A 135      -2.107  17.977  -6.276  1.00 26.88      L111 N
ATOM    958  CA  MET A 135      -2.691  18.308  -7.563  1.00 25.82      L111 C
ATOM    959  C   MET A 135      -2.887  19.801  -7.783  1.00 31.45      L111 C
ATOM    960  O   MET A 135      -3.737  20.209  -8.581  1.00 30.19      L111 O
ATOM    961  CB  MET A 135      -4.029  17.597  -7.711  1.00 27.23      L111 C
ATOM    962  CG  MET A 135      -4.974  17.857  -6.574  1.00 22.80      L111 C
ATOM    963  SD  MET A 135      -6.230  16.597  -6.491  1.00 37.09      L111 S
ATOM    964  CE  MET A 135      -7.008  16.793  -8.089  1.00 41.07      L111 C
ATOM    965  N   GLY A 136      -2.105  20.613  -7.078  1.00 27.82      L111 N
ATOM    966  CA  GLY A 136      -2.215  22.050  -7.228  1.00 22.84      L111 C
ATOM    967  C   GLY A 136      -3.569  22.630  -6.854  1.00 27.99      L111 C
ATOM    968  O   GLY A 136      -4.068  23.538  -7.515  1.00 33.90      L111 O
ATOM    969  N   ILE A 137      -4.181  22.099  -5.806  1.00 27.75      L111 N
ATOM    970  CA  ILE A 137      -5.458  22.621  -5.345  1.00 29.45      L111 C
ATOM    971  C   ILE A 137      -5.207  23.141  -3.934  1.00 37.77      L111 C
ATOM    972  O   ILE A 137      -4.722  22.409  -3.066  1.00 42.44      L111 O
ATOM    973  CB  ILE A 137      -6.553  21.535  -5.334  1.00 29.74      L111 C
ATOM    974  CG1 ILE A 137      -6.755  20.994  -6.751  1.00 30.99      L111 C
ATOM    975  CG2 ILE A 137      -7.864  22.117  -4.842  1.00 21.17      L111 C
ATOM    976  CD1 ILE A 137      -7.883  19.989  -6.877  1.00 23.63      L111 C
ATOM    977  N   GLU A 138      -5.508  24.419  -3.723  1.00 40.79      L111 N
ATOM    978  CA  GLU A 138      -5.299  25.058  -2.435  1.00 39.24      L111 C
ATOM    979  C   GLU A 138      -6.528  25.003  -1.549  1.00 43.73      L111 C
ATOM    980  O   GLU A 138      -7.640  24.799  -2.031  1.00 48.97      L111 O
ATOM    981  CB  GLU A 138      -4.903  26.506  -2.644  1.00 41.53      L111 C
ATOM    982  CG  GLU A 138      -3.466  26.787  -2.294  1.00 59.35      L111 C
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ATOM   983  CD  GLU A 138     -3.094  28.228  -2.556  1.00 67.14      L111 C
ATOM   984  OE1 GLU A 138     -3.950  28.970  -3.098  1.00 59.01      L111 O
ATOM   985  OE2 GLU A 138     -1.950  28.613  -2.220  1.00 67.00      L111 O
ATOM   986  N   VAL A 139     -6.316  25.193  -0.251  1.00 48.03      L111 N
ATOM   987  CA  VAL A 139     -7.404  25.171   0.725  1.00 52.55      L111 C
ATOM   988  C   VAL A 139     -7.561  26.549   1.370  1.00 53.32      L111 C
ATOM   989  O   VAL A 139     -6.578  27.164   1.782  1.00 54.50      L111 O
ATOM   990  CB  VAL A 139     -7.144  24.122   1.838  1.00 47.09      L111 C
ATOM   991  CG1 VAL A 139     -7.486  22.741   1.332  1.00 46.28      L111 C
ATOM   992  CG2 VAL A 139     -5.689  24.171   2.281  1.00 54.07      L111 C
ATOM   993  N   VAL A 140     -8.799  27.028   1.454  1.00 57.53      L111 N
ATOM   994  CA  VAL A 140     -9.076  28.334   2.045  1.00 58.40      L111 C
ATOM   995  C   VAL A 140    -10.295  28.298   2.970  1.00 64.90      L111 C
ATOM   996  O   VAL A 140    -11.243  27.540   2.674  1.00 63.16      L111 O
ATOM   997  CB  VAL A 140     -9.321  29.394   0.950  1.00 56.76      L111 C
ATOM   998  CG1 VAL A 140     -8.207  29.343  -0.082  1.00 48.47      L111 C
ATOM   999  CG2 VAL A 140    -10.667  29.156   0.288  1.00 56.93      L111 C
ATOM  1000  OXT VAL A 140    -10.290  29.036   3.980  1.00 72.53      L111 O
TER   1001      VAL A 140
ATOM  1002  N   LYS B  71    -21.043  -5.854 -42.905  1.00 63.31      L112 N
ATOM  1003  CA  LYS B  71    -20.335  -6.681 -43.925  1.00 62.12      L112 C
ATOM  1004  C   LYS B  71    -20.331  -8.162 -43.563  1.00 64.08      L112 C
ATOM  1005  O   LYS B  71    -20.688  -8.546 -42.446  1.00 64.38      L112 O
ATOM  1006  CB  LYS B  71    -18.892  -6.202 -44.080  1.00 58.09      L112 C
ATOM  1007  CG  LYS B  71    -18.753  -4.928 -44.883  1.00 57.55      L112 C
ATOM  1008  CD  LYS B  71    -17.414  -4.877 -45.584  1.00 59.51      L112 C
ATOM  1009  CE  LYS B  71    -17.502  -4.091 -46.883  1.00 73.52      L112 C
ATOM  1010  NZ  LYS B  71    -16.276  -3.277 -47.136  1.00 74.38      L112 N
ATOM  1011  N   THR B  72    -19.922  -8.992 -44.517  1.00 60.82      L112 N
ATOM  1012  CA  THR B  72    -19.866 -10.432 -44.305  1.00 53.90      L112 C
ATOM  1013  C   THR B  72    -18.602 -10.793 -43.534  1.00 45.75      L112 C
ATOM  1014  O   THR B  72    -17.573 -10.123 -43.661  1.00 42.26      L112 O
ATOM  1015  CB  THR B  72    -19.881 -11.190 -45.647  1.00 54.39      L112 C
ATOM  1016  OG1 THR B  72    -20.261 -10.291 -46.695  1.00 53.11      L112 O
ATOM  1017  CG2 THR B  72    -20.877 -12.340 -45.603  1.00 54.95      L112 C
ATOM  1018  N   PRO B  73    -18.664 -11.860 -42.721  1.00 37.48      L112 N
ATOM  1019  CA  PRO B  73    -17.507 -12.290 -41.935  1.00 34.20      L112 C
ATOM  1020  C   PRO B  73    -16.302 -12.518 -42.828  1.00 36.67      L112 C
ATOM  1021  O   PRO B  73    -16.441 -12.715 -44.034  1.00 42.32      L112 O
ATOM  1022  CB  PRO B  73    -17.977 -13.578 -41.271  1.00 35.95      L112 C
ATOM  1023  CG  PRO B  73    -19.465 -13.478 -41.261  1.00 38.50      L112 C
ATOM  1024  CD  PRO B  73    -19.831 -12.733 -42.504  1.00 38.65      L112 C
ATOM  1025  N   PRO B  74    -15.097 -12.500 -42.247  1.00 30.98      L112 N
ATOM  1026  CA  PRO B  74    -13.896 -12.712 -43.056  1.00 29.22      L112 C
ATOM  1027  C   PRO B  74    -13.949 -14.071 -43.737  1.00 30.46      L112 C
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ATOM 1028 O PRO B 74 -14.664 -14.971 -43.292 1.00 34.58 L112 O
ATOM 1029 CB PRO B 74 -12.755 -12.620 -42.042 1.00 26.89 L112 C
ATOM 1030 CG PRO B 74 -13.334 -11.909 -40.876 1.00 16.14 L112 C
ATOM 1031 CD PRO B 74 -14.773 -12.302 -40.828 1.00 24.82 L112 C
ATOM 1032 N ALA B 75 -13.196 -14.217 -44.819 1.00 26.98 L112 N
ATOM 1033 CA ALA B 75 -13.162 -15.472 -45.540 1.00 21.93 L112 C
ATOM 1034 C ALA B 75 -12.623 -16.534 -44.597 1.00 29.69 L112 C
ATOM 1035 O ALA B 75 -13.190 -17.619 -44.481 1.00 33.14 L112 O
ATOM 1036 CB ALA B 75 -12.264 -15.346 -46.760 1.00 29.99 L112 C
ATOM 1037 N SER B 76 -11.530 -16.210 -43.912 1.00 29.96 L112 N
ATOM 1038 CA SER B 76 -10.911 -17.143 -42.978 1.00 31.14 L112 C
ATOM 1039 C SER B 76 -11.908 -17.595 -41.918 1.00 36.21 L112 C
ATOM 1040 O SER B 76 -11.922 -18.760 -41.517 1.00 38.58 L112 O
ATOM 1041 CB SER B 76 -9.700 -16.496 -42.305 1.00 28.76 L112 C
ATOM 1042 OG SER B 76 -10.103 -15.622 -41.266 1.00 33.61 L112 O
ATOM 1043 N PHE B 77 -12.748 -16.674 -41.465 1.00 35.12 L112 N
ATOM 1044 CA PHE B 77 -13.731 -17.018 -40.457 1.00 36.06 L112 C
ATOM 1045 C PHE B 77 -14.684 -18.047 -41.025 1.00 38.63 L112 C
ATOM 1046 O PHE B 77 -14.874 -19.116 -40.448 1.00 43.61 L112 O
ATOM 1047 CB PHE B 77 -14.518 -15.787 -40.025 1.00 44.62 L112 C
ATOM 1048 CG PHE B 77 -15.644 -16.097 -39.080 1.00 47.58 L112 C
ATOM 1049 CD1 PHE B 77 -15.388 -16.347 -37.733 1.00 44.42 L112 C
ATOM 1050 CD2 PHE B 77 -16.959 -16.151 -39.536 1.00 44.81 L112 C
ATOM 1051 CE1 PHE B 77 -16.424 -16.646 -36.855 1.00 40.74 L112 C
ATOM 1052 CE2 PHE B 77 -18.003 -16.449 -38.667 1.00 42.72 L112 C
ATOM 1053 CZ PHE B 77 -17.736 -16.697 -37.322 1.00 44.82 L112 C
ATOM 1054 N LEU B 78 -15.288 -17.719 -42.161 1.00 37.81 L112 N
ATOM 1055 CA LEU B 78 -16.228 -18.625 -42.810 1.00 36.34 L112 C
ATOM 1056 C LEU B 78 -15.574 -19.970 -43.100 1.00 31.89 L112 C
ATOM 1057 O LEU B 78 -16.204 -21.017 -42.980 1.00 35.90 L112 O
ATOM 1058 CB LEU B 78 -16.743 -17.998 -44.105 1.00 34.71 L112 C
ATOM 1059 CG LEU B 78 -17.603 -16.750 -43.895 1.00 33.80 L112 C
ATOM 1060 CD1 LEU B 78 -18.030 -16.182 -45.238 1.00 29.39 L112 C
ATOM 1061 CD2 LEU B 78 -18.817 -17.113 -43.052 1.00 29.74 L112 C
ATOM 1062 N LEU B 79 -14.302 -19.936 -43.474 1.00 26.28 L112 N
ATOM 1063 CA LEU B 79 -13.566 -21.153 -43.765 1.00 31.61 L112 C
ATOM 1064 C LEU B 79 -13.420 -22.002 -42.498 1.00 39.25 L112 C
ATOM 1065 O LEU B 79 -13.727 -23.194 -42.508 1.00 40.69 L112 O
ATOM 1066 CB LEU B 79 -12.192 -20.799 -44.344 1.00 31.36 L112 C
ATOM 1067 CG LEU B 79 -12.229 -20.369 -45.816 1.00 25.54 L112 C
ATOM 1068 CD1 LEU B 79 -10.852 -19.971 -46.314 1.00 21.73 L112 C
ATOM 1069 CD2 LEU B 79 -12.763 -21.520 -46.635 1.00 23.94 L112 C
ATOM 1070 N LYS B 80 -12.960 -21.384 -41.411 1.00 44.27 L112 N
ATOM 1071 CA LYS B 80 -12.794 -22.078 -40.131 1.00 39.57 L112 C
ATOM 1072 C LYS B 80 -14.075 -22.822 -39.785 1.00 35.79 L112 C

ATOM	1073	O	LYS	B	80	-14.049	-23.993	-39.418	1.00	37.45	L112	O
ATOM	1074	CB	LYS	B	80	-12.500	-21.077	-39.008	1.00	44.26	L112	C
ATOM	1075	CG	LYS	B	80	-11.028	-20.840	-38.710	1.00	46.47	L112	C
ATOM	1076	CD	LYS	B	80	-10.839	-19.591	-37.850	1.00	45.33	L112	C
ATOM	1077	CE	LYS	B	80	-9.377	-19.388	-37.474	1.00	50.24	L112	C
ATOM	1078	NZ	LYS	B	80	-9.071	-17.963	-37.174	1.00	50.61	L112	N
ATOM	1079	N	LYS	B	81	-15.197	-22.122	-39.907	1.00	34.23	L112	N
ATOM	1080	CA	LYS	B	81	-16.508	-22.682	-39.609	1.00	39.48	L112	C
ATOM	1081	C	LYS	B	81	-16.845	-23.880	-40.485	1.00	42.52	L112	C
ATOM	1082	O	LYS	B	81	-17.253	-24.929	-39.991	1.00	49.15	L112	O
ATOM	1083	CB	LYS	B	81	-17.580	-21.607	-39.787	1.00	41.03	L112	C
ATOM	1084	CG	LYS	B	81	-18.306	-21.234	-38.510	1.00	52.41	L112	C
ATOM	1085	CD	LYS	B	81	-19.812	-21.200	-38.730	1.00	68.51	L112	C
ATOM	1086	CE	LYS	B	81	-20.234	-19.983	-39.549	1.00	73.66	L112	C
ATOM	1087	NZ	LYS	B	81	-20.152	-20.217	-41.023	1.00	71.12	L112	N
ATOM	1088	N	ALA	B	82	-16.678	-23.722	-41.792	1.00	45.81	L112	N
ATOM	1089	CA	ALA	B	82	-16.979	-24.800	-42.725	1.00	44.23	L112	C
ATOM	1090	C	ALA	B	82	-16.154	-26.049	-42.431	1.00	40.55	L112	C
ATOM	1091	O	ALA	B	82	-16.662	-27.165	-42.503	1.00	39.77	L112	O
ATOM	1092	CB	ALA	B	82	-16.729	-24.336	-44.149	1.00	42.43	L112	C
ATOM	1093	N	ALA	B	83	-14.882	-25.855	-42.101	1.00	35.34	L112	N
ATOM	1094	CA	ALA	B	83	-13.990	-26.967	-41.807	1.00	33.10	L112	C
ATOM	1095	C	ALA	B	83	-14.259	-27.559	-40.431	1.00	40.90	L112	C
ATOM	1096	O	ALA	B	83	-13.797	-28.659	-40.123	1.00	42.00	L112	O
ATOM	1097	CB	ALA	B	83	-12.544	-26.514	-41.898	1.00	30.83	L112	C
ATOM	1098	N	GLY	B	84	-15.000	-26.823	-39.605	1.00	43.37	L112	N
ATOM	1099	CA	GLY	B	84	-15.320	-27.292	-38.267	1.00	40.61	L112	C
ATOM	1100	C	GLY	B	84	-14.164	-27.194	-37.287	1.00	41.90	L112	C
ATOM	1101	O	GLY	B	84	-14.061	-27.997	-36.361	1.00	45.63	L112	O
ATOM	1102	N	ILE	B	85	-13.283	-26.222	-37.495	1.00	40.72	L112	N
ATOM	1103	CA	ILE	B	85	-12.141	-26.025	-36.612	1.00	39.23	L112	C
ATOM	1104	C	ILE	B	85	-12.283	-24.664	-35.944	1.00	44.21	L112	C
ATOM	1105	O	ILE	B	85	-13.168	-23.884	-36.304	1.00	48.06	L112	O
ATOM	1106	CB	ILE	B	85	-10.801	-26.081	-37.388	1.00	34.91	L112	C
ATOM	1107	CG1	ILE	B	85	-10.738	-24.959	-38.423	1.00	34.57	L112	C
ATOM	1108	CG2	ILE	B	85	-10.657	-27.425	-38.076	1.00	33.20	L112	C
ATOM	1109	CD1	ILE	B	85	-9.477	-24.973	-39.258	1.00	32.16	L112	C
ATOM	1110	N	GLU	B	86	-11.422	-24.380	-34.972	1.00	45.20	L112	N
ATOM	1111	CA	GLU	B	86	-11.484	-23.108	-34.266	1.00	43.68	L112	C
ATOM	1112	C	GLU	B	86	-10.261	-22.245	-34.544	1.00	41.68	L112	C
ATOM	1113	O	GLU	B	86	-10.258	-21.049	-34.257	1.00	47.94	L112	O
ATOM	1114	CB	GLU	B	86	-11.632	-23.347	-32.760	1.00	46.15	L112	C
ATOM	1115	CG	GLU	B	86	-10.322	-23.581	-32.020	1.00	65.68	L112	C
ATOM	1116	CD	GLU	B	86	-10.394	-23.163	-30.561	1.00	76.24	L112	C
ATOM	1117	OE1	GLU	B	86	-11.440	-23.417	-29.922	1.00	79.61	L112	O

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ATOM  1118  OE2 GLU B  86     -9.409 -22.580 -30.054  1.00 77.24      L112 O
ATOM  1119  N   LYS B  87     -9.222 -22.850 -35.103  1.00 33.13      L112 N
ATOM  1120  CA  LYS B  87     -8.011 -22.109 -35.416  1.00 40.07      L112 C
ATOM  1121  C   LYS B  87     -7.423 -22.570 -36.741  1.00 40.26      L112 C
ATOM  1122  O   LYS B  87     -7.610 -23.712 -37.150  1.00 46.66      L112 O
ATOM  1123  CB  LYS B  87     -6.973 -22.293 -34.306  1.00 43.57      L112 C
ATOM  1124  CG  LYS B  87     -7.240 -21.468 -33.057  1.00 57.30      L112 C
ATOM  1125  CD  LYS B  87     -6.210 -21.759 -31.970  1.00 60.56      L112 C
ATOM  1126  CE  LYS B  87     -5.750 -20.483 -31.279  1.00 59.04      L112 C
ATOM  1127  NZ  LYS B  87     -6.112 -19.261 -32.054  1.00 64.31      L112 N
ATOM  1128  N   GLY B  88     -6.725 -21.671 -37.418  1.00 34.46      L112 N
ATOM  1129  CA  GLY B  88     -6.110 -22.038 -38.672  1.00 33.11      L112 C
ATOM  1130  C   GLY B  88     -4.818 -22.742 -38.333  1.00 31.13      L112 C
ATOM  1131  O   GLY B  88     -4.402 -22.747 -37.180  1.00 34.45      L112 O
ATOM  1132  N   SER B  89     -4.183 -23.345 -39.325  1.00 31.44      L112 N
ATOM  1133  CA  SER B  89     -2.935 -24.043 -39.093  1.00 29.45      L112 C
ATOM  1134  C   SER B  89     -1.871 -23.027 -38.709  1.00 37.64      L112 C
ATOM  1135  O   SER B  89     -1.904 -21.889 -39.167  1.00 39.44      L112 O
ATOM  1136  CB  SER B  89     -2.519 -24.789 -40.357  1.00 30.04      L112 C
ATOM  1137  OG  SER B  89     -1.138 -25.097 -40.339  1.00 30.69      L112 O
ATOM  1138  N   SER B  90     -0.932 -23.437 -37.863  1.00 34.79      L112 N
ATOM  1139  CA  SER B  90      0.145 -22.556 -37.434  1.00 36.73      L112 C
ATOM  1140  C   SER B  90      1.250 -22.593 -38.480  1.00 37.59      L112 C
ATOM  1141  O   SER B  90      2.173 -21.778 -38.474  1.00 38.46      L112 O
ATOM  1142  CB  SER B  90      0.698 -23.023 -36.092  1.00 42.80      L112 C
ATOM  1143  OG  SER B  90      1.368 -24.265 -36.234  1.00 57.39      L112 O
ATOM  1144  N   GLU B  91      1.153 -23.565 -39.373  1.00 40.27      L112 N
ATOM  1145  CA  GLU B  91      2.122 -23.726 -40.445  1.00 44.62      L112 C
ATOM  1146  C   GLU B  91      1.352 -24.125 -41.697  1.00 42.72      L112 C
ATOM  1147  O   GLU B  91      1.316 -25.295 -42.067  1.00 49.13      L112 O
ATOM  1148  CB  GLU B  91      3.135 -24.812 -40.085  1.00 47.12      L112 C
ATOM  1149  CG  GLU B  91      4.520 -24.289 -39.768  1.00 58.48      L112 C
ATOM  1150  CD  GLU B  91      5.431 -25.364 -39.208  1.00 65.15      L112 C
ATOM  1151  OE1 GLU B  91      5.935 -26.197 -39.997  1.00 68.92      L112 O
ATOM  1152  OE2 GLU B  91      5.643 -25.374 -37.976  1.00 74.00      L112 O
ATOM  1153  N   PRO B  92      0.699 -23.154 -42.352  1.00 40.19      L112 N
ATOM  1154  CA  PRO B  92     -0.071 -23.435 -43.566  1.00 40.89      L112 C
ATOM  1155  C   PRO B  92      0.736 -24.213 -44.603  1.00 42.71      L112 C
ATOM  1156  O   PRO B  92      1.955 -24.035 -44.720  1.00 32.77      L112 O
ATOM  1157  CB  PRO B  92     -0.467 -22.049 -44.062  1.00 43.77      L112 C
ATOM  1158  CG  PRO B  92     -0.489 -21.217 -42.818  1.00 42.90      L112 C
ATOM  1159  CD  PRO B  92      0.642 -21.729 -41.987  1.00 35.83      L112 C
ATOM  1160  N   LYS B  93      0.043 -25.074 -45.346  1.00 45.71      L112 N
ATOM  1161  CA  LYS B  93      0.656 -25.905 -46.380  1.00 42.76      L112 C
ATOM  1162  C   LYS B  93      1.431 -27.073 -45.773  1.00 42.07      L112 C
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ATOM  1163  O   LYS B  93      1.296 -28.210 -46.223  1.00 47.50      L112 O
ATOM  1164  CB  LYS B  93      1.588 -25.068 -47.267  1.00 46.12      L112 C
ATOM  1165  CG  LYS B  93      1.163 -24.984 -48.735  1.00 52.73      L112 C
ATOM  1166  CD  LYS B  93     -0.145 -24.214 -48.924  1.00 53.15      L112 C
ATOM  1167  CE  LYS B  93      0.025 -23.038 -49.883  1.00 56.74      L112 C
ATOM  1168  NZ  LYS B  93      0.637 -23.435 -51.187  1.00 65.38      L112 N
ATOM  1169  N   ARG B  94      2.232 -26.790 -44.748  1.00 39.69      L112 N
ATOM  1170  CA  ARG B  94      3.028 -27.815 -44.077  1.00 28.33      L112 C
ATOM  1171  C   ARG B  94      2.200 -28.678 -43.134  1.00 27.71      L112 C
ATOM  1172  O   ARG B  94      2.515 -29.841 -42.919  1.00 39.31      L112 O
ATOM  1173  CB  ARG B  94      4.159 -27.172 -43.282  1.00 22.60      L112 C
ATOM  1174  CG  ARG B  94      5.305 -26.668 -44.121  1.00 29.42      L112 C
ATOM  1175  CD  ARG B  94      6.358 -26.019 -43.246  1.00 31.23      L112 C
ATOM  1176  NE  ARG B  94      7.463 -25.486 -44.033  1.00 42.70      L112 N
ATOM  1177  CZ  ARG B  94      8.628 -25.108 -43.516  1.00 56.07      L112 C
ATOM  1178  NH1 ARG B  94      8.833 -25.207 -42.207  1.00 58.35      L112 N
ATOM  1179  NH2 ARG B  94      9.584 -24.628 -44.304  1.00 57.97      L112 N
ATOM  1180  N   LYS B  95      1.146 -28.110 -42.568  1.00 27.38      L112 N
ATOM  1181  CA  LYS B  95      0.301 -28.850 -41.645  1.00 29.34      L112 C
ATOM  1182  C   LYS B  95     -1.150 -28.482 -41.891  1.00 30.96      L112 C
ATOM  1183  O   LYS B  95     -1.551 -27.342 -41.680  1.00 36.81      L112 O
ATOM  1184  CB  LYS B  95      0.688 -28.513 -40.200  1.00 39.33      L112 C
ATOM  1185  CG  LYS B  95      0.177 -29.500 -39.158  1.00 54.73      L112 C
ATOM  1186  CD  LYS B  95     -0.879 -28.870 -38.249  1.00 67.65      L112 C
ATOM  1187  CE  LYS B  95     -0.393 -28.746 -36.801  1.00 74.12      L112 C
ATOM  1188  NZ  LYS B  95     -0.959 -27.548 -36.096  1.00 63.57      L112 N
ATOM  1189  N   ILE B  96     -1.937 -29.446 -42.345  1.00 32.10      L112 N
ATOM  1190  CA  ILE B  96     -3.347 -29.195 -42.614  1.00 32.15      L112 C
ATOM  1191  C   ILE B  96     -4.165 -29.436 -41.353  1.00 33.56      L112 C
ATOM  1192  O   ILE B  96     -4.075 -30.496 -40.739  1.00 42.84      L112 O
ATOM  1193  CB  ILE B  96     -3.863 -30.103 -43.759  1.00 28.05      L112 C
ATOM  1194  CG1 ILE B  96     -3.017 -29.876 -45.014  1.00 11.50      L112 C
ATOM  1195  CG2 ILE B  96     -5.330 -29.814 -44.048  1.00 19.38      L112 C
ATOM  1196  CD1 ILE B  96     -2.904 -28.429 -45.429  1.00 19.93      L112 C
ATOM  1197  N   VAL B  97     -4.964 -28.448 -40.973  1.00 32.84      L112 N
ATOM  1198  CA  VAL B  97     -5.776 -28.552 -39.770  1.00 29.62      L112 C
ATOM  1199  C   VAL B  97     -7.232 -28.853 -40.066  1.00 29.20      L112 C
ATOM  1200  O   VAL B  97     -8.015 -29.112 -39.156  1.00 36.19      L112 O
ATOM  1201  CB  VAL B  97     -5.717 -27.246 -38.949  1.00 28.85      L112 C
ATOM  1202  CG1 VAL B  97     -4.288 -26.945 -38.556  1.00 28.11      L112 C
ATOM  1203  CG2 VAL B  97     -6.291 -26.094 -39.760  1.00 28.49      L112 C
ATOM  1204  N   GLY B  98     -7.605 -28.811 -41.337  1.00 34.31      L112 N
ATOM  1205  CA  GLY B  98     -8.988 -29.072 -41.685  1.00 28.21      L112 C
ATOM  1206  C   GLY B  98     -9.152 -29.147 -43.181  1.00 30.18      L112 C
ATOM  1207  O   GLY B  98     -8.192 -28.965 -43.923  1.00 30.67      L112 O
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ATOM  1208  N   LYS B  99    -10.373 -29.402 -43.627  1.00 29.50      L112 N
ATOM  1209  CA  LYS B  99    -10.634 -29.516 -45.046  1.00 32.51      L112 C
ATOM  1210  C   LYS B  99    -12.080 -29.187 -45.374  1.00 36.44      L112 C
ATOM  1211  O   LYS B  99    -12.976 -29.448 -44.575  1.00 35.95      L112 O
ATOM  1212  CB  LYS B  99    -10.315 -30.937 -45.507  1.00 39.97      L112 C
ATOM  1213  CG  LYS B  99    -10.933 -32.025 -44.639  1.00 41.83      L112 C
ATOM  1214  CD  LYS B  99    -11.335 -33.237 -45.469  1.00 51.41      L112 C
ATOM  1215  CE  LYS B  99    -10.486 -34.453 -45.134  1.00 53.02      L112 C
ATOM  1216  NZ  LYS B  99    -11.298 -35.553 -44.538  1.00 66.17      L112 N
ATOM  1217  N   VAL B 100    -12.298 -28.609 -46.555  1.00 40.79      L112 N
ATOM  1218  CA  VAL B 100    -13.642 -28.263 -47.010  1.00 40.95      L112 C
ATOM  1219  C   VAL B 100    -13.871 -28.788 -48.419  1.00 41.23      L112 C
ATOM  1220  O   VAL B 100    -12.927 -28.948 -49.199  1.00 37.76      L112 O
ATOM  1221  CB  VAL B 100    -13.877 -26.742 -47.033  1.00 42.14      L112 C
ATOM  1222  CG1 VAL B 100    -14.062 -26.228 -45.623  1.00 47.48      L112 C
ATOM  1223  CG2 VAL B 100    -12.714 -26.049 -47.719  1.00 46.52      L112 C
ATOM  1224  N   THR B 101    -15.134 -29.054 -48.737  1.00 43.68      L112 N
ATOM  1225  CA  THR B 101    -15.505 -29.556 -50.052  1.00 44.90      L112 C
ATOM  1226  C   THR B 101    -15.572 -28.401 -51.030  1.00 46.97      L112 C
ATOM  1227  O   THR B 101    -15.847 -27.266 -50.641  1.00 49.23      L112 O
ATOM  1228  CB  THR B 101    -16.882 -30.228 -50.037  1.00 44.59      L112 C
ATOM  1229  OG1 THR B 101    -17.875 -29.262 -49.670  1.00 47.42      L112 O
ATOM  1230  CG2 THR B 101    -16.904 -31.382 -49.050  1.00 37.18      L112 C
ATOM  1231  N   ARG B 102    -15.319 -28.692 -52.301  1.00 47.23      L112 N
ATOM  1232  CA  ARG B 102    -15.376 -27.664 -53.324  1.00 42.99      L112 C
ATOM  1233  C   ARG B 102    -16.760 -27.046 -53.255  1.00 39.27      L112 C
ATOM  1234  O   ARG B 102    -16.947 -25.888 -53.609  1.00 51.83      L112 O
ATOM  1235  CB  ARG B 102    -15.140 -28.272 -54.708  1.00 50.12      L112 C
ATOM  1236  CG  ARG B 102    -14.295 -27.405 -55.639  1.00 58.67      L112 C
ATOM  1237  CD  ARG B 102    -12.884 -27.964 -55.821  1.00 61.68      L112 C
ATOM  1238  NE  ARG B 102    -12.827 -29.413 -55.632  1.00 63.94      L112 N
ATOM  1239  CZ  ARG B 102    -11.703 -30.124 -55.623  1.00 67.71      L112 C
ATOM  1240  NH1 ARG B 102    -10.534 -29.517 -55.793  1.00 66.40      L112 N
ATOM  1241  NH2 ARG B 102    -11.747 -31.442 -55.443  1.00 60.88      L112 N
ATOM  1242  N   LYS B 103    -17.730 -27.823 -52.786  1.00 37.67      L112 N
ATOM  1243  CA  LYS B 103    -19.096 -27.333 -52.664  1.00 41.92      L112 C
ATOM  1244  C   LYS B 103    -19.160 -26.308 -51.547  1.00 44.83      L112 C
ATOM  1245  O   LYS B 103    -19.856 -25.298 -51.649  1.00 49.24      L112 O
ATOM  1246  CB  LYS B 103    -20.056 -28.483 -52.354  1.00 49.35      L112 C
ATOM  1247  CG  LYS B 103    -21.265 -28.079 -51.510  1.00 57.47      L112 C
ATOM  1248  CD  LYS B 103    -22.244 -27.221 -52.298  1.00 66.45      L112 C
ATOM  1249  CE  LYS B 103    -23.683 -27.670 -52.075  1.00 76.17      L112 C
ATOM  1250  NZ  LYS B 103    -24.099 -27.557 -50.645  1.00 75.72      L112 N
ATOM  1251  N   GLN B 104    -18.434 -26.578 -50.471  1.00 44.97      L112 N
ATOM  1252  CA  GLN B 104    -18.412 -25.662 -49.347  1.00 43.50      L112 C
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ATOM  1253  C   GLN B 104    -17.766 -24.359 -49.796  1.00 37.68      L112 C
ATOM  1254  O   GLN B 104    -18.268 -23.277 -49.500  1.00 38.95      L112 O
ATOM  1255  CB  GLN B 104    -17.640 -26.279 -48.181  1.00 47.34      L112 C
ATOM  1256  CG  GLN B 104    -18.442 -27.328 -47.425  1.00 42.38      L112 C
ATOM  1257  CD  GLN B 104    -17.693 -27.890 -46.237  1.00 42.53      L112 C
ATOM  1258  OE1 GLN B 104    -16.603 -28.446 -46.380  1.00 35.56      L112 O
ATOM  1259  NE2 GLN B 104    -18.275 -27.745 -45.050  1.00 36.61      L112 N
ATOM  1260  N   ILE B 105    -16.660 -24.471 -50.525  1.00 30.76      L112 N
ATOM  1261  CA  ILE B 105    -15.962 -23.296 -51.026  1.00 35.17      L112 C
ATOM  1262  C   ILE B 105    -16.931 -22.427 -51.811  1.00 39.38      L112 C
ATOM  1263  O   ILE B 105    -16.880 -21.202 -51.736  1.00 44.28      L112 O
ATOM  1264  CB  ILE B 105    -14.808 -23.678 -51.962  1.00 26.23      L112 C
ATOM  1265  CG1 ILE B 105    -13.674 -24.314 -51.159  1.00 35.32      L112 C
ATOM  1266  CG2 ILE B 105    -14.320 -22.442 -52.714  1.00 30.76      L112 C
ATOM  1267  CD1 ILE B 105    -12.778 -23.317 -50.444  1.00 30.65      L112 C
ATOM  1268  N   GLU B 106    -17.815 -23.074 -52.563  1.00 44.23      L112 N
ATOM  1269  CA  GLU B 106    -18.800 -22.367 -53.366  1.00 48.57      L112 C
ATOM  1270  C   GLU B 106    -19.776 -21.590 -52.488  1.00 50.45      L112 C
ATOM  1271  O   GLU B 106    -20.083 -20.430 -52.769  1.00 52.09      L112 O
ATOM  1272  CB  GLU B 106    -19.563 -23.358 -54.249  1.00 56.57      L112 C
ATOM  1273  CG  GLU B 106    -20.814 -22.786 -54.920  1.00 65.87      L112 C
ATOM  1274  CD  GLU B 106    -21.335 -23.664 -56.053  1.00 68.27      L112 C
ATOM  1275  OE1 GLU B 106    -20.505 -24.254 -56.781  1.00 62.09      L112 O
ATOM  1276  OE2 GLU B 106    -22.573 -23.762 -56.214  1.00 66.69      L112 O
ATOM  1277  N   GLU B 107    -20.258 -22.222 -51.422  1.00 48.38      L112 N
ATOM  1278  CA  GLU B 107    -21.204 -21.567 -50.523  1.00 50.26      L112 C
ATOM  1279  C   GLU B 107    -20.610 -20.317 -49.890  1.00 50.25      L112 C
ATOM  1280  O   GLU B 107    -21.311 -19.332 -49.661  1.00 52.98      L112 O
ATOM  1281  CB  GLU B 107    -21.648 -22.527 -49.425  1.00 52.51      L112 C
ATOM  1282  CG  GLU B 107    -22.481 -23.685 -49.921  1.00 72.08      L112 C
ATOM  1283  CD  GLU B 107    -22.371 -24.896 -49.016  1.00 86.41      L112 C
ATOM  1284  OE1 GLU B 107    -21.249 -25.188 -48.545  1.00 91.57      L112 O
ATOM  1285  OE2 GLU B 107    -23.405 -25.554 -48.772  1.00 92.70      L112 O
ATOM  1286  N   ILE B 108    -19.315 -20.355 -49.602  1.00 46.38      L112 N
ATOM  1287  CA  ILE B 108    -18.667 -19.206 -48.999  1.00 43.09      L112 C
ATOM  1288  C   ILE B 108    -18.525 -18.099 -50.030  1.00 42.47      L112 C
ATOM  1289  O   ILE B 108    -18.815 -16.937 -49.748  1.00 47.10      L112 O
ATOM  1290  CB  ILE B 108    -17.272 -19.565 -48.449  1.00 42.76      L112 C
ATOM  1291  CG1 ILE B 108    -17.407 -20.613 -47.345  1.00 35.09      L112 C
ATOM  1292  CG2 ILE B 108    -16.592 -18.317 -47.891  1.00 31.13      L112 C
ATOM  1293  CD1 ILE B 108    -16.084 -21.041 -46.747  1.00 41.11      L112 C
ATOM  1294  N   ALA B 109    -18.081 -18.464 -51.229  1.00 38.62      L112 N
ATOM  1295  CA  ALA B 109    -17.900 -17.486 -52.293  1.00 38.24      L112 C
ATOM  1296  C   ALA B 109    -19.208 -16.761 -52.539  1.00 37.79      L112 C
ATOM  1297  O   ALA B 109    -19.222 -15.562 -52.807  1.00 37.18      L112 O
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ATOM 1298 CB ALA B 109 -17.436 -18.172 -53.562 1.00 38.10 L112 C
ATOM 1299 N LYS B 110 -20.309 -17.497 -52.437 1.00 38.29 L112 N
ATOM 1300 CA LYS B 110 -21.626 -16.917 -52.647 1.00 42.58 L112 C
ATOM 1301 C LYS B 110 -21.945 -15.951 -51.518 1.00 45.99 L112 C
ATOM 1302 O LYS B 110 -22.468 -14.858 -51.747 1.00 55.26 L112 O
ATOM 1303 CB LYS B 110 -22.689 -18.016 -52.702 1.00 39.40 L112 C
ATOM 1304 CG LYS B 110 -22.558 -18.947 -53.898 1.00 51.26 L112 C
ATOM 1305 CD LYS B 110 -23.911 -19.512 -54.329 1.00 60.46 L112 C
ATOM 1306 CE LYS B 110 -23.897 -19.968 -55.790 1.00 63.75 L112 C
ATOM 1307 NZ LYS B 110 -24.464 -21.340 -55.985 1.00 64.25 L112 N
ATOM 1308 N THR B 111 -21.620 -16.357 -50.297 1.00 40.79 L112 N
ATOM 1309 CA THR B 111 -21.876 -15.527 -49.134 1.00 38.24 L112 C
ATOM 1310 C THR B 111 -21.088 -14.231 -49.196 1.00 42.37 L112 C
ATOM 1311 O THR B 111 -21.644 -13.152 -48.998 1.00 48.64 L112 O
ATOM 1312 CB THR B 111 -21.490 -16.256 -47.845 1.00 42.62 L112 C
ATOM 1313 OG1 THR B 111 -22.140 -17.531 -47.812 1.00 49.22 L112 O
ATOM 1314 CG2 THR B 111 -21.899 -15.441 -46.630 1.00 41.08 L112 C
ATOM 1315 N LYS B 112 -19.794 -14.346 -49.479 1.00 41.09 L112 N
ATOM 1316 CA LYS B 112 -18.900 -13.194 -49.544 1.00 38.50 L112 C
ATOM 1317 C LYS B 112 -18.910 -12.449 -50.879 1.00 43.09 L112 C
ATOM 1318 O LYS B 112 -18.246 -11.424 -51.018 1.00 40.13 L112 O
ATOM 1319 CB LYS B 112 -17.467 -13.640 -49.240 1.00 35.11 L112 C
ATOM 1320 CG LYS B 112 -17.124 -13.715 -47.764 1.00 33.43 L112 C
ATOM 1321 CD LYS B 112 -16.011 -12.742 -47.409 1.00 29.28 L112 C
ATOM 1322 CE LYS B 112 -16.567 -11.530 -46.680 1.00 35.42 L112 C
ATOM 1323 NZ LYS B 112 -15.524 -10.509 -46.385 1.00 31.34 L112 N
ATOM 1324 N MET B 113 -19.654 -12.957 -51.857 1.00 50.88 L112 N
ATOM 1325 CA MET B 113 -19.709 -12.331 -53.180 1.00 51.11 L112 C
ATOM 1326 C MET B 113 -19.879 -10.807 -53.156 1.00 49.15 L112 C
ATOM 1327 O MET B 113 -19.130 -10.081 -53.813 1.00 50.15 L112 O
ATOM 1328 CB MET B 113 -20.824 -12.962 -54.022 1.00 51.18 L112 C
ATOM 1329 CG MET B 113 -20.717 -12.654 -55.515 1.00 47.98 L112 C
ATOM 1330 SD MET B 113 -19.263 -13.400 -56.298 1.00 49.73 L112 S
ATOM 1331 CE MET B 113 -18.549 -11.969 -57.088 1.00 52.43 L112 C
ATOM 1332 N PRO B 114 -20.870 -10.301 -52.409 1.00 42.31 L112 N
ATOM 1333 CA PRO B 114 -21.051 -8.849 -52.369 1.00 41.88 L112 C
ATOM 1334 C PRO B 114 -19.781 -8.079 -51.997 1.00 44.88 L112 C
ATOM 1335 O PRO B 114 -19.589 -6.945 -52.439 1.00 51.97 L112 O
ATOM 1336 CB PRO B 114 -22.171 -8.646 -51.345 1.00 38.22 L112 C
ATOM 1337 CG PRO B 114 -22.290 -9.946 -50.621 1.00 43.79 L112 C
ATOM 1338 CD PRO B 114 -21.870 -11.000 -51.588 1.00 46.66 L112 C
ATOM 1339 N ASP B 115 -18.912 -8.690 -51.197 1.00 46.07 L112 N
ATOM 1340 CA ASP B 115 -17.673 -8.030 -50.785 1.00 45.61 L112 C
ATOM 1341 C ASP B 115 -16.506 -8.353 -51.709 1.00 42.88 L112 C
ATOM 1342 O ASP B 115 -15.435 -7.758 -51.598 1.00 47.89 L112 O

ATOM	1343	CB	ASP	B	115	-17.292	-8.429	-49.355	1.00	51.51	L112	C
ATOM	1344	CG	ASP	B	115	-18.431	-8.252	-48.368	1.00	50.88	L112	C
ATOM	1345	OD1	ASP	B	115	-19.514	-7.787	-48.779	1.00	57.98	L112	O
ATOM	1346	OD2	ASP	B	115	-18.240	-8.582	-47.178	1.00	59.37	L112	O
ATOM	1347	N	LEU	B	116	-16.713	-9.298	-52.618	1.00	40.70	L112	N
ATOM	1348	CA	LEU	B	116	-15.669	-9.698	-53.553	1.00	37.46	L112	C
ATOM	1349	C	LEU	B	116	-15.698	-8.849	-54.819	1.00	37.00	L112	C
ATOM	1350	O	LEU	B	116	-16.757	-8.385	-55.242	1.00	38.81	L112	O
ATOM	1351	CB	LEU	B	116	-15.851	-11.169	-53.939	1.00	40.60	L112	C
ATOM	1352	CG	LEU	B	116	-15.289	-12.293	-53.065	1.00	35.62	L112	C
ATOM	1353	CD1	LEU	B	116	-14.872	-11.765	-51.707	1.00	42.51	L112	C
ATOM	1354	CD2	LEU	B	116	-16.347	-13.368	-52.923	1.00	33.28	L112	C
ATOM	1355	N	ASN	B	117	-14.535	-8.653	-55.429	1.00	32.39	L112	N
ATOM	1356	CA	ASN	B	117	-14.467	-7.886	-56.662	1.00	32.20	L112	C
ATOM	1357	C	ASN	B	117	-14.427	-8.835	-57.867	1.00	37.64	L112	C
ATOM	1358	O	ASN	B	117	-14.193	-8.415	-59.001	1.00	35.01	L112	O
ATOM	1359	CB	ASN	B	117	-13.235	-6.984	-56.655	1.00	24.31	L112	C
ATOM	1360	CG	ASN	B	117	-11.952	-7.762	-56.709	1.00	29.72	L112	C
ATOM	1361	OD1	ASN	B	117	-11.914	-8.941	-56.354	1.00	32.78	L112	O
ATOM	1362	ND2	ASN	B	117	-10.883	-7.110	-57.154	1.00	25.55	L112	N
ATOM	1363	N	ALA	B	118	-14.662	-10.117	-57.608	1.00	39.75	L112	N
ATOM	1364	CA	ALA	B	118	-14.665	-11.130	-58.656	1.00	41.80	L112	C
ATOM	1365	C	ALA	B	118	-15.862	-10.910	-59.567	1.00	45.30	L112	C
ATOM	1366	O	ALA	B	118	-16.863	-10.330	-59.156	1.00	53.58	L112	O
ATOM	1367	CB	ALA	B	118	-14.734	-12.512	-58.043	1.00	30.65	L112	C
ATOM	1368	N	ASN	B	119	-15.760	-11.381	-60.804	1.00	46.03	L112	N
ATOM	1369	CA	ASN	B	119	-16.840	-11.216	-61.766	1.00	48.46	L112	C
ATOM	1370	C	ASN	B	119	-17.574	-12.516	-62.081	1.00	50.16	L112	C
ATOM	1371	O	ASN	B	119	-18.557	-12.512	-62.817	1.00	55.94	L112	O
ATOM	1372	CB	ASN	B	119	-16.287	-10.625	-63.061	1.00	49.26	L112	C
ATOM	1373	CG	ASN	B	119	-16.023	-9.137	-62.958	1.00	50.05	L112	C
ATOM	1374	OD1	ASN	B	119	-16.747	-8.407	-62.269	1.00	48.95	L112	O
ATOM	1375	ND2	ASN	B	119	-14.981	-8.674	-63.646	1.00	48.05	L112	N
ATOM	1376	N	SER	B	120	-17.096	-13.624	-61.527	1.00	51.92	L112	N
ATOM	1377	CA	SER	B	120	-17.711	-14.924	-61.771	1.00	47.70	L112	C
ATOM	1378	C	SER	B	120	-17.599	-15.828	-60.555	1.00	50.21	L112	C
ATOM	1379	O	SER	B	120	-16.614	-15.770	-59.823	1.00	58.54	L112	O
ATOM	1380	CB	SER	B	120	-17.034	-15.609	-62.964	1.00	46.48	L112	C
ATOM	1381	OG	SER	B	120	-15.617	-15.558	-62.866	1.00	29.64	L112	O
ATOM	1382	N	LEU	B	121	-18.607	-16.670	-60.346	1.00	49.76	L112	N
ATOM	1383	CA	LEU	B	121	-18.591	-17.600	-59.225	1.00	44.29	L112	C
ATOM	1384	C	LEU	B	121	-17.276	-18.369	-59.261	1.00	42.13	L112	C
ATOM	1385	O	LEU	B	121	-16.669	-18.628	-58.229	1.00	45.70	L112	O
ATOM	1386	CB	LEU	B	121	-19.760	-18.578	-59.327	1.00	41.45	L112	C
ATOM	1387	CG	LEU	B	121	-19.784	-19.676	-58.262	1.00	41.89	L112	C

ATOM	1388	CD1	LEU	B	121	-19.585	-19.051	-56.890	1.00	40.55	L112	C
ATOM	1389	CD2	LEU	B	121	-21.102	-20.431	-58.320	1.00	32.73	L112	C
ATOM	1390	N	GLU	B	122	-16.842	-18.722	-60.465	1.00	39.88	L112	N
ATOM	1391	CA	GLU	B	122	-15.593	-19.447	-60.666	1.00	40.08	L112	C
ATOM	1392	C	GLU	B	122	-14.444	-18.620	-60.091	1.00	38.04	L112	C
ATOM	1393	O	GLU	B	122	-13.606	-19.135	-59.355	1.00	43.79	L112	O
ATOM	1394	CB	GLU	B	122	-15.377	-19.699	-62.170	1.00	47.41	L112	C
ATOM	1395	CG	GLU	B	122	-14.120	-20.496	-62.548	1.00	66.40	L112	C
ATOM	1396	CD	GLU	B	122	-14.105	-20.935	-64.023	1.00	79.56	L112	C
ATOM	1397	OE1	GLU	B	122	-15.061	-21.614	-64.461	1.00	83.56	L112	O
ATOM	1398	OE2	GLU	B	122	-13.137	-20.604	-64.747	1.00	80.21	L112	O
ATOM	1399	N	ALA	B	123	-14.416	-17.332	-60.422	1.00	37.15	L112	N
ATOM	1400	CA	ALA	B	123	-13.369	-16.432	-59.946	1.00	31.33	L112	C
ATOM	1401	C	ALA	B	123	-13.466	-16.220	-58.440	1.00	32.49	L112	C
ATOM	1402	O	ALA	B	123	-12.458	-16.207	-57.736	1.00	32.50	L112	O
ATOM	1403	CB	ALA	B	123	-13.472	-15.096	-60.655	1.00	28.73	L112	C
ATOM	1404	N	ALA	B	124	-14.689	-16.042	-57.958	1.00	26.80	L112	N
ATOM	1405	CA	ALA	B	124	-14.937	-15.835	-56.545	1.00	22.39	L112	C
ATOM	1406	C	ALA	B	124	-14.365	-16.994	-55.736	1.00	30.24	L112	C
ATOM	1407	O	ALA	B	124	-13.632	-16.790	-54.773	1.00	32.38	L112	O
ATOM	1408	CB	ALA	B	124	-16.434	-15.714	-56.304	1.00	19.73	L112	C
ATOM	1409	N	MET	B	125	-14.695	-18.214	-56.147	1.00	38.83	L112	N
ATOM	1410	CA	MET	B	125	-14.232	-19.422	-55.468	1.00	34.24	L112	C
ATOM	1411	C	MET	B	125	-12.718	-19.546	-55.464	1.00	30.68	L112	C
ATOM	1412	O	MET	B	125	-12.142	-20.147	-54.562	1.00	39.64	L112	O
ATOM	1413	CB	MET	B	125	-14.839	-20.659	-56.125	1.00	37.17	L112	C
ATOM	1414	CG	MET	B	125	-16.346	-20.783	-55.948	1.00	34.83	L112	C
ATOM	1415	SD	MET	B	125	-16.993	-22.386	-56.480	1.00	44.61	L112	S
ATOM	1416	CE	MET	B	125	-15.586	-23.063	-57.397	1.00	33.28	L112	C
ATOM	1417	N	LYS	B	126	-12.074	-18.991	-56.480	1.00	26.30	L112	N
ATOM	1418	CA	LYS	B	126	-10.622	-19.038	-56.558	1.00	27.93	L112	C
ATOM	1419	C	LYS	B	126	-10.072	-18.083	-55.503	1.00	30.79	L112	C
ATOM	1420	O	LYS	B	126	-8.932	-18.220	-55.056	1.00	35.96	L112	O
ATOM	1421	CB	LYS	B	126	-10.146	-18.601	-57.946	1.00	32.20	L112	C
ATOM	1422	CG	LYS	B	126	-10.107	-19.703	-58.994	1.00	27.48	L112	C
ATOM	1423	CD	LYS	B	126	-8.844	-19.598	-59.850	1.00	40.52	L112	C
ATOM	1424	CE	LYS	B	126	-9.159	-19.142	-61.268	1.00	32.95	L112	C
ATOM	1425	NZ	LYS	B	126	-9.919	-20.188	-62.011	1.00	51.40	L112	N
ATOM	1426	N	ILE	B	127	-10.895	-17.110	-55.114	1.00	31.30	L112	N
ATOM	1427	CA	ILE	B	127	-10.511	-16.117	-54.111	1.00	30.96	L112	C
ATOM	1428	C	ILE	B	127	-10.523	-16.741	-52.718	1.00	28.53	L112	C
ATOM	1429	O	ILE	B	127	-9.570	-16.587	-51.952	1.00	27.30	L112	O
ATOM	1430	CB	ILE	B	127	-11.469	-14.899	-54.139	1.00	27.50	L112	C
ATOM	1431	CG1	ILE	B	127	-11.203	-14.064	-55.391	1.00	29.44	L112	C
ATOM	1432	CG2	ILE	B	127	-11.268	-14.038	-52.902	1.00	28.00	L112	C

ATOM 1433 CD1 ILE B 127 -12.047 -12.810 -55.482 1.00 31.68 L112 C
ATOM 1434 N ILE B 128 -11.608 -17.439 -52.396 1.00 20.75 L112 N
ATOM 1435 CA ILE B 128 -11.731 -18.104 -51.111 1.00 18.60 L112 C
ATOM 1436 C ILE B 128 -10.637 -19.152 -50.969 1.00 23.21 L112 C
ATOM 1437 O ILE B 128 -9.936 -19.202 -49.960 1.00 34.11 L112 O
ATOM 1438 CB ILE B 128 -13.084 -18.796 -50.975 1.00 17.63 L112 C
ATOM 1439 CG1 ILE B 128 -14.208 -17.807 -51.280 1.00 17.94 L112 C
ATOM 1440 CG2 ILE B 128 -13.236 -19.348 -49.581 1.00 23.67 L112 C
ATOM 1441 CD1 ILE B 128 -14.138 -16.529 -50.469 1.00 20.35 L112 C
ATOM 1442 N GLU B 129 -10.488 -19.985 -51.989 1.00 23.93 L112 N
ATOM 1443 CA GLU B 129 -9.473 -21.025 -51.982 1.00 27.79 L112 C
ATOM 1444 C GLU B 129 -8.116 -20.447 -51.612 1.00 28.96 L112 C
ATOM 1445 O GLU B 129 -7.332 -21.079 -50.907 1.00 34.08 L112 O
ATOM 1446 CB GLU B 129 -9.379 -21.666 -53.359 1.00 43.68 L112 C
ATOM 1447 CG GLU B 129 -9.007 -23.129 -53.344 1.00 54.25 L112 C
ATOM 1448 CD GLU B 129 -9.708 -23.894 -54.445 1.00 67.26 L112 C
ATOM 1449 OE1 GLU B 129 -10.697 -23.356 -54.998 1.00 58.57 L112 O
ATOM 1450 OE2 GLU B 129 -9.272 -25.027 -54.754 1.00 76.46 L112 O
ATOM 1451 N GLY B 130 -7.836 -19.248 -52.108 1.00 29.13 L112 N
ATOM 1452 CA GLY B 130 -6.571 -18.609 -51.809 1.00 23.84 L112 C
ATOM 1453 C GLY B 130 -6.440 -18.423 -50.315 1.00 27.27 L112 C
ATOM 1454 O GLY B 130 -5.372 -18.629 -49.735 1.00 29.16 L112 O
ATOM 1455 N THR B 131 -7.536 -18.031 -49.680 1.00 19.93 L112 N
ATOM 1456 CA THR B 131 -7.521 -17.839 -48.242 1.00 27.52 L112 C
ATOM 1457 C THR B 131 -7.337 -19.204 -47.579 1.00 28.05 L112 C
ATOM 1458 O THR B 131 -6.453 -19.383 -46.741 1.00 33.97 L112 O
ATOM 1459 CB THR B 131 -8.832 -17.187 -47.758 1.00 25.95 L112 C
ATOM 1460 OG1 THR B 131 -8.954 -15.883 -48.335 1.00 19.66 L112 O
ATOM 1461 CG2 THR B 131 -8.836 -17.050 -46.255 1.00 29.87 L112 C
ATOM 1462 N ALA B 132 -8.164 -20.167 -47.977 1.00 23.92 L112 N
ATOM 1463 CA ALA B 132 -8.101 -21.523 -47.436 1.00 21.36 L112 C
ATOM 1464 C ALA B 132 -6.704 -22.108 -47.505 1.00 21.61 L112 C
ATOM 1465 O ALA B 132 -6.253 -22.768 -46.575 1.00 34.50 L112 O
ATOM 1466 CB ALA B 132 -9.060 -22.428 -48.182 1.00 19.47 L112 C
ATOM 1467 N LYS B 133 -6.015 -21.870 -48.610 1.00 25.84 L112 N
ATOM 1468 CA LYS B 133 -4.674 -22.405 -48.779 1.00 29.20 L112 C
ATOM 1469 C LYS B 133 -3.693 -21.721 -47.851 1.00 27.88 L112 C
ATOM 1470 O LYS B 133 -2.642 -22.270 -47.530 1.00 37.04 L112 O
ATOM 1471 CB LYS B 133 -4.213 -22.232 -50.230 1.00 33.18 L112 C
ATOM 1472 CG LYS B 133 -5.011 -23.052 -51.235 1.00 37.46 L112 C
ATOM 1473 CD LYS B 133 -4.884 -22.487 -52.640 1.00 50.67 L112 C
ATOM 1474 CE LYS B 133 -3.636 -23.010 -53.343 1.00 51.75 L112 C
ATOM 1475 NZ LYS B 133 -3.389 -22.329 -54.654 1.00 54.53 L112 N
ATOM 1476 N SER B 134 -4.042 -20.518 -47.416 1.00 36.66 L112 N
ATOM 1477 CA SER B 134 -3.168 -19.747 -46.539 1.00 36.64 L112 C

ATOM 1478 C SER B 134 -3.344 -20.080 -45.066 1.00 33.11 L112 C
ATOM 1479 O SER B 134 -2.635 -19.541 -44.223 1.00 37.50 L112 O
ATOM 1480 CB SER B 134 -3.414 -18.252 -46.741 1.00 34.18 L112 C
ATOM 1481 OG SER B 134 -4.603 -17.857 -46.080 1.00 23.48 L112 O
ATOM 1482 N MET B 135 -4.281 -20.964 -44.748 1.00 29.84 L112 N
ATOM 1483 CA MET B 135 -4.509 -21.312 -43.357 1.00 23.70 L112 C
ATOM 1484 C MET B 135 -4.602 -22.808 -43.089 1.00 29.55 L112 C
ATOM 1485 O MET B 135 -5.283 -23.242 -42.161 1.00 23.32 L112 O
ATOM 1486 CB MET B 135 -5.768 -20.618 -42.857 1.00 22.94 L112 C
ATOM 1487 CG MET B 135 -7.034 -21.139 -43.448 1.00 17.81 L112 C
ATOM 1488 SD MET B 135 -8.303 -19.898 -43.327 1.00 34.08 L112 S
ATOM 1489 CE MET B 135 -9.264 -20.525 -41.959 1.00 35.79 L112 C
ATOM 1490 N GLY B 136 -3.914 -23.592 -43.910 1.00 35.43 L112 N
ATOM 1491 CA GLY B 136 -3.911 -25.030 -43.728 1.00 27.07 L112 C
ATOM 1492 C GLY B 136 -5.245 -25.737 -43.854 1.00 28.44 L112 C
ATOM 1493 O GLY B 136 -5.524 -26.683 -43.120 1.00 30.60 L112 O
ATOM 1494 N ILE B 137 -6.088 -25.289 -44.770 1.00 27.95 L112 N
ATOM 1495 CA ILE B 137 -7.357 -25.966 -44.963 1.00 31.48 L112 C
ATOM 1496 C ILE B 137 -7.358 -26.505 -46.389 1.00 36.97 L112 C
ATOM 1497 O ILE B 137 -7.192 -25.752 -47.350 1.00 43.45 L112 O
ATOM 1498 CB ILE B 137 -8.547 -25.019 -44.736 1.00 31.35 L112 C
ATOM 1499 CG1 ILE B 137 -8.702 -24.756 -43.233 1.00 30.66 L112 C
ATOM 1500 CG2 ILE B 137 -9.826 -25.634 -45.302 1.00 23.26 L112 C
ATOM 1501 CD1 ILE B 137 -9.853 -23.843 -42.859 1.00 19.47 L112 C
ATOM 1502 N GLU B 138 -7.516 -27.820 -46.508 1.00 34.70 L112 N
ATOM 1503 CA GLU B 138 -7.523 -28.504 -47.793 1.00 24.78 L112 C
ATOM 1504 C GLU B 138 -8.909 -28.509 -48.402 1.00 30.83 L112 C
ATOM 1505 O GLU B 138 -9.911 -28.509 -47.685 1.00 25.06 L112 O
ATOM 1506 CB GLU B 138 -7.065 -29.949 -47.617 1.00 33.57 L112 C
ATOM 1507 CG GLU B 138 -5.717 -30.270 -48.240 1.00 53.60 L112 C
ATOM 1508 CD GLU B 138 -5.435 -31.769 -48.293 1.00 61.48 L112 C
ATOM 1509 OE1 GLU B 138 -6.286 -32.555 -47.810 1.00 52.54 L112 O
ATOM 1510 OE2 GLU B 138 -4.359 -32.152 -48.818 1.00 61.92 L112 O
ATOM 1511 N VAL B 139 -8.962 -28.518 -49.733 1.00 36.08 L112 N
ATOM 1512 CA VAL B 139 -10.234 -28.552 -50.450 1.00 32.76 L112 C
ATOM 1513 C VAL B 139 -10.392 -29.933 -51.077 1.00 35.50 L112 C
ATOM 1514 O VAL B 139 -9.434 -30.484 -51.624 1.00 35.56 L112 O
ATOM 1515 CB VAL B 139 -10.293 -27.477 -51.557 1.00 24.66 L112 C
ATOM 1516 CG1 VAL B 139 -11.653 -27.507 -52.234 1.00 22.09 L112 C
ATOM 1517 CG2 VAL B 139 -10.044 -26.102 -50.959 1.00 19.96 L112 C
ATOM 1518 N VAL B 140 -11.593 -30.499 -50.978 1.00 39.97 L112 N
ATOM 1519 CA VAL B 140 -11.862 -31.825 -51.534 1.00 47.65 L112 C
ATOM 1520 C VAL B 140 -13.287 -31.934 -52.091 1.00 51.84 L112 C
ATOM 1521 O VAL B 140 -13.610 -32.955 -52.740 1.00 48.50 L112 O
ATOM 1522 CB VAL B 140 -11.651 -32.933 -50.467 1.00 46.88 L112 C

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ATOM  1523  CG1 VAL B 140     -11.479 -34.280 -51.152  1.00 53.45      L112 C
ATOM  1524  CG2 VAL B 140     -10.421 -32.628 -49.615  1.00 37.90      L112 C
ATOM  1525  OXT VAL B 140     -14.071 -30.988 -51.877  1.00 56.26      L112 O
TER   1526      VAL B 140
ATOM  1527  O5*   G C1051      24.335 -12.173   6.313  1.00 73.26      RNA1 O
ATOM  1528  C5*   G C1051      22.929 -12.367   6.147  1.00 60.23      RNA1 C
ATOM  1529  C4*   G C1051      22.454 -13.612   6.854  1.00 60.92      RNA1 C
ATOM  1530  O4*   G C1051      22.709 -13.474   8.275  1.00 63.63      RNA1 O
ATOM  1531  C3*   G C1051      20.961 -13.878   6.747  1.00 62.37      RNA1 C
ATOM  1532  O3*   G C1051      20.640 -14.594   5.557  1.00 56.24      RNA1 O
ATOM  1533  C2*   G C1051      20.665 -14.668   8.018  1.00 60.79      RNA1 C
ATOM  1534  O2*   G C1051      20.939 -16.050   7.900  1.00 63.11      RNA1 O
ATOM  1535  C1*   G C1051      21.637 -14.032   9.016  1.00 57.61      RNA1 C
ATOM  1536  N9    G C1051      21.014 -12.959   9.786  1.00 54.68      RNA1 N
ATOM  1537  C8    G C1051      21.204 -11.607   9.624  1.00 57.52      RNA1 C
ATOM  1538  N7    G C1051      20.474 -10.887  10.430  1.00 63.57      RNA1 N
ATOM  1539  C5    G C1051      19.766 -11.817  11.176  1.00 60.31      RNA1 C
ATOM  1540  C6    G C1051      18.808 -11.631  12.205  1.00 65.69      RNA1 C
ATOM  1541  O6    G C1051      18.372 -10.568  12.669  1.00 71.42      RNA1 O
ATOM  1542  N1    G C1051      18.347 -12.847  12.698  1.00 61.97      RNA1 N
ATOM  1543  C2    G C1051      18.751 -14.081  12.257  1.00 58.15      RNA1 C
ATOM  1544  N2    G C1051      18.193 -15.135  12.861  1.00 61.86      RNA1 N
ATOM  1545  N3    G C1051      19.636 -14.269  11.294  1.00 58.41      RNA1 N
ATOM  1546  C4    G C1051      20.099 -13.101  10.802  1.00 56.62      RNA1 C
ATOM  1547  P     C C1052      19.126 -14.611   5.015  1.00 50.79      RNA1 P
ATOM  1548  O1P   C C1052      18.620 -13.217   4.973  1.00 58.55      RNA1 O
ATOM  1549  O2P   C C1052      19.094 -15.438   3.784  1.00 67.52      RNA1 O
ATOM  1550  O5*   C C1052      18.323 -15.374   6.155  1.00 48.31      RNA1 O
ATOM  1551  C5*   C C1052      18.502 -16.781   6.372  1.00 35.63      RNA1 C
ATOM  1552  C4*   C C1052      17.510 -17.267   7.392  1.00 38.42      RNA1 C
ATOM  1553  O4*   C C1052      17.824 -16.686   8.682  1.00 47.16      RNA1 O
ATOM  1554  C3*   C C1052      16.087 -16.825   7.117  1.00 44.09      RNA1 C
ATOM  1555  O3*   C C1052      15.438 -17.673   6.200  1.00 49.32      RNA1 O
ATOM  1556  C2*   C C1052      15.449 -16.814   8.499  1.00 46.87      RNA1 C
ATOM  1557  O2*   C C1052      14.978 -18.071   8.935  1.00 46.62      RNA1 O
ATOM  1558  C1*   C C1052      16.623 -16.360   9.368  1.00 48.30      RNA1 C
ATOM  1559  N1    C C1052      16.588 -14.902   9.601  1.00 47.59      RNA1 N
ATOM  1560  C2    C C1052      15.778 -14.405  10.629  1.00 47.88      RNA1 C
ATOM  1561  O2    C C1052      15.145 -15.205  11.338  1.00 45.47      RNA1 O
ATOM  1562  N3    C C1052      15.706 -13.069  10.824  1.00 51.51      RNA1 N
ATOM  1563  C4    C C1052      16.406 -12.242  10.045  1.00 47.87      RNA1 C
ATOM  1564  N4    C C1052      16.289 -10.929  10.263  1.00 45.35      RNA1 N
ATOM  1565  C5    C C1052      17.252 -12.720   9.006  1.00 42.28      RNA1 C
ATOM  1566  C6    C C1052      17.314 -14.043   8.821  1.00 43.16      RNA1 C
ATOM  1567  P     U C1053      14.314 -17.067   5.236  1.00 53.77      RNA1 P
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ATOM 1568 O1P U C1053 14.776 -15.724 4.784 1.00 61.48 RNA1 O
ATOM 1569 O2P U C1053 13.984 -18.106 4.231 1.00 67.30 RNA1 O
ATOM 1570 O5* U C1053 13.059 -16.888 6.196 1.00 51.10 RNA1 O
ATOM 1571 C5* U C1053 12.448 -18.032 6.809 1.00 47.98 RNA1 C
ATOM 1572 C4* U C1053 11.467 -17.603 7.868 1.00 47.08 RNA1 C
ATOM 1573 O4* U C1053 12.170 -16.895 8.917 1.00 48.31 RNA1 O
ATOM 1574 C3* U C1053 10.382 -16.641 7.423 1.00 49.60 RNA1 C
ATOM 1575 O3* U C1053 9.295 -17.321 6.812 1.00 61.44 RNA1 O
ATOM 1576 C2* U C1053 9.993 -15.961 8.730 1.00 50.47 RNA1 C
ATOM 1577 O2* U C1053 9.119 -16.731 9.531 1.00 43.66 RNA1 O
ATOM 1578 C1* U C1053 11.339 -15.875 9.443 1.00 44.87 RNA1 C
ATOM 1579 N1 U C1053 12.003 -14.575 9.247 1.00 55.73 RNA1 N
ATOM 1580 C2 U C1053 11.564 -13.505 10.018 1.00 53.37 RNA1 C
ATOM 1581 O2 U C1053 10.644 -13.591 10.824 1.00 47.71 RNA1 O
ATOM 1582 N3 U C1053 12.240 -12.328 9.807 1.00 43.32 RNA1 N
ATOM 1583 C4 U C1053 13.281 -12.110 8.928 1.00 42.60 RNA1 C
ATOM 1584 O4 U C1053 13.827 -11.008 8.906 1.00 44.05 RNA1 O
ATOM 1585 C5 U C1053 13.666 -13.253 8.157 1.00 39.63 RNA1 C
ATOM 1586 C6 U C1053 13.032 -14.415 8.336 1.00 51.41 RNA1 C
ATOM 1587 P G C1054 8.426 -16.576 5.682 1.00 62.77 RNA1 P
ATOM 1588 O1P G C1054 9.391 -15.966 4.732 1.00 48.23 RNA1 O
ATOM 1589 O2P G C1054 7.391 -17.524 5.177 1.00 63.46 RNA1 O
ATOM 1590 O5* G C1054 7.673 -15.417 6.482 1.00 57.93 RNA1 O
ATOM 1591 C5* G C1054 6.589 -15.737 7.376 1.00 58.01 RNA1 C
ATOM 1592 C4* G C1054 6.160 -14.521 8.162 1.00 54.61 RNA1 C
ATOM 1593 O4* G C1054 7.279 -14.019 8.937 1.00 57.89 RNA1 O
ATOM 1594 C3* G C1054 5.693 -13.296 7.392 1.00 56.27 RNA1 C
ATOM 1595 O3* G C1054 4.352 -13.378 6.946 1.00 61.66 RNA1 O
ATOM 1596 C2* G C1054 5.851 -12.189 8.425 1.00 52.95 RNA1 C
ATOM 1597 O2* G C1054 4.779 -12.130 9.346 1.00 49.43 RNA1 O
ATOM 1598 C1* G C1054 7.119 -12.626 9.148 1.00 47.41 RNA1 C
ATOM 1599 N9 G C1054 8.274 -11.911 8.616 1.00 41.21 RNA1 N
ATOM 1600 C8 G C1054 9.205 -12.347 7.703 1.00 35.70 RNA1 C
ATOM 1601 N7 G C1054 10.100 -11.440 7.414 1.00 39.32 RNA1 N
ATOM 1602 C5 G C1054 9.741 -10.342 8.190 1.00 34.83 RNA1 C
ATOM 1603 C6 G C1054 10.333 -9.051 8.304 1.00 30.48 RNA1 C
ATOM 1604 O6 G C1054 11.333 -8.604 7.728 1.00 27.46 RNA1 O
ATOM 1605 N1 G C1054 9.635 -8.245 9.199 1.00 30.56 RNA1 N
ATOM 1606 C2 G C1054 8.511 -8.623 9.898 1.00 43.91 RNA1 C
ATOM 1607 N2 G C1054 7.967 -7.703 10.717 1.00 37.62 RNA1 N
ATOM 1608 N3 G C1054 7.957 -9.818 9.803 1.00 43.41 RNA1 N
ATOM 1609 C4 G C1054 8.619 -10.620 8.938 1.00 41.38 RNA1 C
ATOM 1610 P G C1055 3.878 -12.469 5.704 1.00 66.88 RNA1 P
ATOM 1611 O1P G C1055 4.889 -12.575 4.612 1.00 48.03 RNA1 O
ATOM 1612 O2P G C1055 2.452 -12.820 5.440 1.00 64.70 RNA1 O

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ATOM  1613  O5*  G C1055      3.943 -10.971   6.248  1.00 63.61      RNA1 O
ATOM  1614  C5*  G C1055      3.012 -10.512   7.237  1.00 53.95      RNA1 C
ATOM  1615  C4*  G C1055      3.371  -9.125   7.706  1.00 46.33      RNA1 C
ATOM  1616  O4*  G C1055      4.737  -9.107   8.201  1.00 45.69      RNA1 O
ATOM  1617  C3*  G C1055      3.363  -8.001   6.687  1.00 40.52      RNA1 C
ATOM  1618  O3*  G C1055      2.066  -7.500   6.421  1.00 47.06      RNA1 O
ATOM  1619  C2*  G C1055      4.212  -6.943   7.377  1.00 42.04      RNA1 C
ATOM  1620  O2*  G C1055      3.475  -6.224   8.348  1.00 43.70      RNA1 O
ATOM  1621  C1*  G C1055      5.264  -7.798   8.076  1.00 31.41      RNA1 C
ATOM  1622  N9   G C1055      6.501  -7.839   7.307  1.00 24.39      RNA1 N
ATOM  1623  C8   G C1055      7.026  -8.888   6.592  1.00 29.37      RNA1 C
ATOM  1624  N7   G C1055      8.158  -8.591   6.005  1.00 32.88      RNA1 N
ATOM  1625  C5   G C1055      8.388  -7.266   6.352  1.00 23.47      RNA1 C
ATOM  1626  C6   G C1055      9.458  -6.393   6.013  1.00 28.67      RNA1 C
ATOM  1627  O6   G C1055     10.450  -6.622   5.314  1.00 27.35      RNA1 O
ATOM  1628  N1   G C1055      9.292  -5.136   6.584  1.00 24.95      RNA1 N
ATOM  1629  C2   G C1055      8.235  -4.763   7.377  1.00 26.92      RNA1 C
ATOM  1630  N2   G C1055      8.255  -3.513   7.838  1.00 28.71      RNA1 N
ATOM  1631  N3   G C1055      7.234  -5.561   7.696  1.00 22.90      RNA1 N
ATOM  1632  C4   G C1055      7.375  -6.789   7.155  1.00 29.13      RNA1 C
ATOM  1633  P    G C1056      1.758  -6.834   4.989  1.00 49.25      RNA1 P
ATOM  1634  O1P  G C1056      1.991  -7.883   3.963  1.00 42.81      RNA1 O
ATOM  1635  O2P  G C1056      0.428  -6.158   5.065  1.00 37.09      RNA1 O
ATOM  1636  O5*  G C1056      2.899  -5.734   4.819  1.00 32.92      RNA1 O
ATOM  1637  C5*  G C1056      2.796  -4.457   5.476  1.00 35.07      RNA1 C
ATOM  1638  C4*  G C1056      3.939  -3.563   5.065  1.00 31.58      RNA1 C
ATOM  1639  O4*  G C1056      5.187  -4.183   5.457  1.00 35.44      RNA1 O
ATOM  1640  C3*  G C1056      4.089  -3.329   3.575  1.00 34.14      RNA1 C
ATOM  1641  O3*  G C1056      3.270  -2.275   3.113  1.00 39.89      RNA1 O
ATOM  1642  C2*  G C1056      5.567  -3.005   3.429  1.00 33.87      RNA1 C
ATOM  1643  O2*  G C1056      5.865  -1.651   3.704  1.00 36.26      RNA1 O
ATOM  1644  C1*  G C1056      6.184  -3.915   4.489  1.00 31.52      RNA1 C
ATOM  1645  N9   G C1056      6.611  -5.191   3.922  1.00 35.38      RNA1 N
ATOM  1646  C8   G C1056      5.874  -6.350   3.845  1.00 33.57      RNA1 C
ATOM  1647  N7   G C1056      6.516  -7.326   3.265  1.00 40.73      RNA1 N
ATOM  1648  C5   G C1056      7.752  -6.782   2.941  1.00 37.74      RNA1 C
ATOM  1649  C6   G C1056      8.875  -7.367   2.290  1.00 41.95      RNA1 C
ATOM  1650  O6   G C1056      8.999  -8.519   1.852  1.00 52.67      RNA1 O
ATOM  1651  N1   G C1056      9.925  -6.460   2.169  1.00 34.10      RNA1 N
ATOM  1652  C2   G C1056      9.899  -5.160   2.611  1.00 28.22      RNA1 C
ATOM  1653  N2   G C1056     11.011  -4.444   2.407  1.00 29.23      RNA1 N
ATOM  1654  N3   G C1056      8.860  -4.603   3.211  1.00 30.05      RNA1 N
ATOM  1655  C4   G C1056      7.829  -5.466   3.344  1.00 33.38      RNA1 C
ATOM  1656  P    A C1057      2.647  -2.350   1.636  1.00 36.51      RNA1 P
ATOM  1657  O1P  A C1057      2.944  -1.053   0.973  1.00 50.45      RNA1 O
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ATOM	1658	O2P	A	C1057	3.064	-3.614	0.988	1.00	31.54	RNA1	O
ATOM	1659	O5*	A	C1057	1.085	-2.420	1.900	1.00	24.51	RNA1	O
ATOM	1660	C5*	A	C1057	0.516	-3.490	2.659	1.00	23.76	RNA1	C
ATOM	1661	C4*	A	C1057	-0.421	-2.936	3.703	1.00	25.17	RNA1	C
ATOM	1662	O4*	A	C1057	0.346	-2.384	4.802	1.00	26.26	RNA1	O
ATOM	1663	C3*	A	C1057	-1.282	-1.776	3.240	1.00	26.38	RNA1	C
ATOM	1664	O3*	A	C1057	-2.429	-2.174	2.517	1.00	39.01	RNA1	O
ATOM	1665	C2*	A	C1057	-1.612	-1.068	4.542	1.00	23.04	RNA1	C
ATOM	1666	O2*	A	C1057	-2.658	-1.705	5.241	1.00	26.68	RNA1	O
ATOM	1667	C1*	A	C1057	-0.304	-1.230	5.310	1.00	20.72	RNA1	C
ATOM	1668	N9	A	C1057	0.587	-0.081	5.125	1.00	25.31	RNA1	N
ATOM	1669	C8	A	C1057	1.840	-0.055	4.550	1.00	24.58	RNA1	C
ATOM	1670	N7	A	C1057	2.393	1.135	4.537	1.00	16.48	RNA1	N
ATOM	1671	C5	A	C1057	1.445	1.949	5.143	1.00	18.96	RNA1	C
ATOM	1672	C6	A	C1057	1.428	3.322	5.438	1.00	21.91	RNA1	C
ATOM	1673	N6	A	C1057	2.445	4.150	5.174	1.00	18.97	RNA1	N
ATOM	1674	N1	A	C1057	0.322	3.824	6.029	1.00	28.79	RNA1	N
ATOM	1675	C2	A	C1057	-0.688	2.991	6.317	1.00	26.99	RNA1	C
ATOM	1676	N3	A	C1057	-0.786	1.681	6.104	1.00	27.54	RNA1	N
ATOM	1677	C4	A	C1057	0.326	1.215	5.505	1.00	19.03	RNA1	C
ATOM	1678	P	U	C1058	-2.943	-1.256	1.300	1.00	33.80	RNA1	P
ATOM	1679	O1P	U	C1058	-1.733	-0.731	0.608	1.00	32.34	RNA1	O
ATOM	1680	O2P	U	C1058	-3.967	-1.996	0.524	1.00	30.00	RNA1	O
ATOM	1681	O5*	U	C1058	-3.665	-0.043	2.030	1.00	29.35	RNA1	O
ATOM	1682	C5*	U	C1058	-4.955	-0.218	2.627	1.00	31.01	RNA1	C
ATOM	1683	C4*	U	C1058	-5.530	1.120	3.008	1.00	33.02	RNA1	C
ATOM	1684	O4*	U	C1058	-4.686	1.734	4.018	1.00	32.59	RNA1	O
ATOM	1685	C3*	U	C1058	-5.554	2.156	1.902	1.00	34.36	RNA1	C
ATOM	1686	O3*	U	C1058	-6.626	2.018	0.993	1.00	36.65	RNA1	O
ATOM	1687	C2*	U	C1058	-5.596	3.459	2.680	1.00	27.20	RNA1	C
ATOM	1688	O2*	U	C1058	-6.886	3.727	3.188	1.00	26.74	RNA1	O
ATOM	1689	C1*	U	C1058	-4.652	3.139	3.831	1.00	24.15	RNA1	C
ATOM	1690	N1	U	C1058	-3.267	3.546	3.532	1.00	18.02	RNA1	N
ATOM	1691	C2	U	C1058	-2.971	4.898	3.590	1.00	19.91	RNA1	C
ATOM	1692	O2	U	C1058	-3.802	5.750	3.879	1.00	30.16	RNA1	O
ATOM	1693	N3	U	C1058	-1.671	5.219	3.300	1.00	13.57	RNA1	N
ATOM	1694	C4	U	C1058	-0.655	4.353	2.965	1.00	20.26	RNA1	C
ATOM	1695	O4	U	C1058	0.470	4.801	2.729	1.00	30.19	RNA1	O
ATOM	1696	C5	U	C1058	-1.035	2.981	2.926	1.00	12.30	RNA1	C
ATOM	1697	C6	U	C1058	-2.296	2.631	3.205	1.00	13.08	RNA1	C
ATOM	1698	P	G	C1059	-6.470	2.631	-0.484	1.00	30.00	RNA1	P
ATOM	1699	O1P	G	C1059	-5.071	2.397	-0.938	1.00	16.05	RNA1	O
ATOM	1700	O2P	G	C1059	-7.607	2.157	-1.311	1.00	33.73	RNA1	O
ATOM	1701	O5*	G	C1059	-6.635	4.196	-0.256	1.00	30.83	RNA1	O
ATOM	1702	C5*	G	C1059	-7.854	4.731	0.279	1.00	22.74	RNA1	C

ATOM	1703	C4*	G C1059	-7.798	6.231	0.278	1.00	24.79	RNA1 C
ATOM	1704	O4*	G C1059	-6.727	6.667	1.149	1.00	28.49	RNA1 O
ATOM	1705	C3*	G C1059	-7.475	6.869	-1.060	1.00	26.72	RNA1 C
ATOM	1706	O3*	G C1059	-8.642	7.007	-1.857	1.00	34.13	RNA1 O
ATOM	1707	C2*	G C1059	-6.884	8.214	-0.657	1.00	28.17	RNA1 C
ATOM	1708	O2*	G C1059	-7.880	9.178	-0.371	1.00	38.10	RNA1 O
ATOM	1709	C1*	G C1059	-6.157	7.860	0.640	1.00	23.13	RNA1 C
ATOM	1710	N9	G C1059	-4.721	7.665	0.480	1.00	15.04	RNA1 N
ATOM	1711	C8	G C1059	-4.064	6.490	0.206	1.00	17.72	RNA1 C
ATOM	1712	N7	G C1059	-2.766	6.634	0.130	1.00	21.45	RNA1 N
ATOM	1713	C5	G C1059	-2.552	7.989	0.360	1.00	9.82	RNA1 C
ATOM	1714	C6	G C1059	-1.344	8.740	0.392	1.00	23.72	RNA1 C
ATOM	1715	O6	G C1059	-0.177	8.344	0.216	1.00	19.54	RNA1 O
ATOM	1716	N1	G C1059	-1.585	10.082	0.661	1.00	19.14	RNA1 N
ATOM	1717	C2	G C1059	-2.822	10.638	0.874	1.00	19.08	RNA1 C
ATOM	1718	N2	G C1059	-2.837	11.957	1.125	1.00	16.35	RNA1 N
ATOM	1719	N3	G C1059	-3.955	9.953	0.844	1.00	20.08	RNA1 N
ATOM	1720	C4	G C1059	-3.746	8.641	0.582	1.00	20.00	RNA1 C
ATOM	1721	P	U C1060	-8.509	7.045	-3.456	1.00	31.42	RNA1 P
ATOM	1722	O1P	U C1060	-9.692	6.330	-3.996	1.00	31.37	RNA1 O
ATOM	1723	O2P	U C1060	-8.243	8.446	-3.872	1.00	36.54	RNA1 O
ATOM	1724	O5*	U C1060	-7.195	6.198	-3.754	1.00	22.64	RNA1 O
ATOM	1725	C5*	U C1060	-7.016	5.523	-5.009	1.00	22.76	RNA1 C
ATOM	1726	C4*	U C1060	-5.589	5.064	-5.145	1.00	18.28	RNA1 C
ATOM	1727	O4*	U C1060	-4.739	6.232	-5.160	1.00	20.83	RNA1 O
ATOM	1728	C3*	U C1060	-5.079	4.166	-4.022	1.00	28.38	RNA1 C
ATOM	1729	O3*	U C1060	-4.142	3.234	-4.559	1.00	34.99	RNA1 O
ATOM	1730	C2*	U C1060	-4.336	5.141	-3.110	1.00	28.41	RNA1 C
ATOM	1731	O2*	U C1060	-3.277	4.523	-2.401	1.00	41.53	RNA1 O
ATOM	1732	C1*	U C1060	-3.794	6.157	-4.115	1.00	23.82	RNA1 C
ATOM	1733	N1	U C1060	-3.613	7.518	-3.587	1.00	15.63	RNA1 N
ATOM	1734	C2	U C1060	-2.336	7.922	-3.245	1.00	18.51	RNA1 C
ATOM	1735	O2	U C1060	-1.353	7.193	-3.325	1.00	21.06	RNA1 O
ATOM	1736	N3	U C1060	-2.245	9.216	-2.800	1.00	13.56	RNA1 N
ATOM	1737	C4	U C1060	-3.271	10.129	-2.661	1.00	21.90	RNA1 C
ATOM	1738	O4	U C1060	-3.015	11.281	-2.293	1.00	25.73	RNA1 O
ATOM	1739	C5	U C1060	-4.559	9.632	-3.018	1.00	7.65	RNA1 C
ATOM	1740	C6	U C1060	-4.686	8.377	-3.455	1.00	23.41	RNA1 C
ATOM	1741	P	U C1061	-4.622	2.136	-5.633	1.00	28.90	RNA1 P
ATOM	1742	O1P	U C1061	-3.994	0.840	-5.253	1.00	34.87	RNA1 O
ATOM	1743	O2P	U C1061	-6.093	2.222	-5.792	1.00	16.57	RNA1 O
ATOM	1744	O5*	U C1061	-3.946	2.631	-6.983	1.00	24.02	RNA1 O
ATOM	1745	C5*	U C1061	-2.514	2.667	-7.117	1.00	25.58	RNA1 C
ATOM	1746	C4*	U C1061	-2.122	3.503	-8.311	1.00	31.26	RNA1 C
ATOM	1747	O4*	U C1061	-2.694	2.914	-9.507	1.00	36.66	RNA1 O

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ATOM  1748  C3*  U C1061     -2.584   4.961  -8.290  1.00 33.14      RNA1 C
ATOM  1749  O3*  U C1061     -1.601   5.740  -8.967  1.00 23.50      RNA1 O
ATOM  1750  C2*  U C1061     -3.831   4.934  -9.167  1.00 32.29      RNA1 C
ATOM  1751  O2*  U C1061     -4.100   6.183  -9.775  1.00 33.30      RNA1 O
ATOM  1752  C1*  U C1061     -3.414   3.896 -10.205  1.00 40.61      RNA1 C
ATOM  1753  N1   U C1061     -4.461   3.257 -11.015  1.00 50.51      RNA1 N
ATOM  1754  C2   U C1061     -4.299   3.335 -12.387  1.00 62.28      RNA1 C
ATOM  1755  O2   U C1061     -3.330   3.880 -12.914  1.00 62.30      RNA1 O
ATOM  1756  N3   U C1061     -5.303   2.754 -13.123  1.00 73.69      RNA1 N
ATOM  1757  C4   U C1061     -6.427   2.110 -12.641  1.00 67.10      RNA1 C
ATOM  1758  O4   U C1061     -7.260   1.668 -13.440  1.00 68.66      RNA1 O
ATOM  1759  C5   U C1061     -6.515   2.056 -11.210  1.00 54.52      RNA1 C
ATOM  1760  C6   U C1061     -5.552   2.617 -10.463  1.00 45.73      RNA1 C
ATOM  1761  P    G C1062     -0.570   6.637  -8.138  1.00 27.54      RNA1 P
ATOM  1762  O1P  G C1062     -0.356   5.986  -6.813  1.00 24.54      RNA1 O
ATOM  1763  O2P  G C1062      0.600   6.908  -9.017  1.00 15.00      RNA1 O
ATOM  1764  O5*  G C1062     -1.358   8.001  -7.930  1.00 14.13      RNA1 O
ATOM  1765  C5*  G C1062     -2.396   8.125  -6.939  1.00 22.88      RNA1 C
ATOM  1766  C4*  G C1062     -2.448   9.547  -6.435  1.00 15.45      RNA1 C
ATOM  1767  O4*  G C1062     -1.246   9.824  -5.677  1.00 24.75      RNA1 O
ATOM  1768  C3*  G C1062     -2.438  10.568  -7.550  1.00 12.59      RNA1 C
ATOM  1769  O3*  G C1062     -3.742  10.823  -8.006  1.00 33.25      RNA1 O
ATOM  1770  C2*  G C1062     -1.783  11.777  -6.911  1.00 19.71      RNA1 C
ATOM  1771  O2*  G C1062     -2.709  12.520  -6.141  1.00 23.78      RNA1 O
ATOM  1772  C1*  G C1062     -0.751  11.111  -5.999  1.00 16.39      RNA1 C
ATOM  1773  N9   G C1062      0.564  10.927  -6.611  1.00 14.13      RNA1 N
ATOM  1774  C8   G C1062      1.229   9.734  -6.776  1.00 24.14      RNA1 C
ATOM  1775  N7   G C1062      2.388   9.866  -7.361  1.00 25.47      RNA1 N
ATOM  1776  C5   G C1062      2.495  11.229  -7.605  1.00 26.26      RNA1 C
ATOM  1777  C6   G C1062      3.527  11.966  -8.235  1.00 31.66      RNA1 C
ATOM  1778  O6   G C1062      4.572  11.542  -8.758  1.00 28.31      RNA1 O
ATOM  1779  N1   G C1062      3.246  13.328  -8.243  1.00 23.22      RNA1 N
ATOM  1780  C2   G C1062      2.108  13.904  -7.739  1.00 23.93      RNA1 C
ATOM  1781  N2   G C1062      2.025  15.238  -7.844  1.00 18.71      RNA1 N
ATOM  1782  N3   G C1062      1.125  13.226  -7.174  1.00 19.22      RNA1 N
ATOM  1783  C4   G C1062      1.384  11.902  -7.137  1.00 21.18      RNA1 C
ATOM  1784  P    G C1063     -3.983  11.091  -9.564  1.00 32.90      RNA1 P
ATOM  1785  O1P  G C1063     -3.162  10.105 -10.324  1.00 29.07      RNA1 O
ATOM  1786  O2P  G C1063     -5.446  11.159  -9.776  1.00 28.95      RNA1 O
ATOM  1787  O5*  G C1063     -3.361  12.534  -9.798  1.00 32.11      RNA1 O
ATOM  1788  C5*  G C1063     -4.042  13.712  -9.342  1.00 23.86      RNA1 C
ATOM  1789  C4*  G C1063     -3.302  14.944  -9.798  1.00 22.38      RNA1 C
ATOM  1790  O4*  G C1063     -1.983  14.950  -9.201  1.00 24.88      RNA1 O
ATOM  1791  C3*  G C1063     -3.019  15.022 -11.287  1.00 26.89      RNA1 C
ATOM  1792  O3*  G C1063     -4.110  15.506 -12.042  1.00 33.17      RNA1 O
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ATOM  1793  C2*  G C1063     -1.806  15.936 -11.343  1.00 25.82      RNA1 C
ATOM  1794  O2*  G C1063     -2.149  17.294 -11.168  1.00 34.75      RNA1 O
ATOM  1795  C1*  G C1063     -1.035  15.472 -10.118  1.00 14.96      RNA1 C
ATOM  1796  N9   G C1063     -0.093  14.412 -10.461  1.00 16.28      RNA1 N
ATOM  1797  C8   G C1063     -0.201  13.070 -10.178  1.00 17.00      RNA1 C
ATOM  1798  N7   G C1063      0.820  12.373 -10.602  1.00 23.95      RNA1 N
ATOM  1799  C5   G C1063      1.644  13.309 -11.212  1.00 13.66      RNA1 C
ATOM  1800  C6   G C1063      2.898  13.151 -11.857  1.00 19.46      RNA1 C
ATOM  1801  O6   G C1063      3.555  12.117 -12.032  1.00 27.29      RNA1 O
ATOM  1802  N1   G C1063      3.385  14.363 -12.326  1.00 19.82      RNA1 N
ATOM  1803  C2   G C1063      2.749  15.571 -12.201  1.00 24.09      RNA1 C
ATOM  1804  N2   G C1063      3.385  16.631 -12.718  1.00 33.27      RNA1 N
ATOM  1805  N3   G C1063      1.579  15.731 -11.609  1.00 25.48      RNA1 N
ATOM  1806  C4   G C1063      1.091  14.569 -11.137  1.00 16.05      RNA1 C
ATOM  1807  P    C C1064     -4.385  14.882 -13.495  1.00 32.63      RNA1 P
ATOM  1808  O1P  C C1064     -4.311  13.399 -13.376  1.00 34.14      RNA1 O
ATOM  1809  O2P  C C1064     -5.610  15.520 -14.047  1.00 34.53      RNA1 O
ATOM  1810  O5*  C C1064     -3.124  15.351 -14.340  1.00 25.39      RNA1 O
ATOM  1811  C5*  C C1064     -2.841  16.743 -14.483  1.00 20.47      RNA1 C
ATOM  1812  C4*  C C1064     -1.510  16.945 -15.158  1.00 22.15      RNA1 C
ATOM  1813  O4*  C C1064     -0.455  16.348 -14.362  1.00 25.83      RNA1 O
ATOM  1814  C3*  C C1064     -1.320  16.321 -16.528  1.00 29.48      RNA1 C
ATOM  1815  O3*  C C1064     -1.921  17.088 -17.565  1.00 35.84      RNA1 O
ATOM  1816  C2*  C C1064      0.199  16.267 -16.648  1.00 29.04      RNA1 C
ATOM  1817  O2*  C C1064      0.774  17.500 -17.036  1.00 28.73      RNA1 O
ATOM  1818  C1*  C C1064      0.611  15.958 -15.212  1.00 21.28      RNA1 C
ATOM  1819  N1   C C1064      0.899  14.525 -15.020  1.00 19.09      RNA1 N
ATOM  1820  C2   C C1064      2.155  14.044 -15.409  1.00 27.83      RNA1 C
ATOM  1821  O2   C C1064      2.977  14.836 -15.897  1.00 32.73      RNA1 O
ATOM  1822  N3   C C1064      2.442  12.734 -15.247  1.00 23.67      RNA1 N
ATOM  1823  C4   C C1064      1.535  11.915 -14.716  1.00 22.40      RNA1 C
ATOM  1824  N4   C C1064      1.871  10.635 -14.564  1.00 29.03      RNA1 N
ATOM  1825  C5   C C1064      0.246  12.374 -14.314  1.00  9.70      RNA1 C
ATOM  1826  C6   C C1064     -0.027  13.674 -14.482  1.00 20.34      RNA1 C
ATOM  1827  P    U C1065     -2.537  16.339 -18.853  1.00 31.56      RNA1 P
ATOM  1828  O1P  U C1065     -3.488  15.293 -18.407  1.00 29.35      RNA1 O
ATOM  1829  O2P  U C1065     -3.011  17.398 -19.774  1.00 46.70      RNA1 O
ATOM  1830  O5*  U C1065     -1.266  15.617 -19.495  1.00 22.04      RNA1 O
ATOM  1831  C5*  U C1065     -0.138  16.392 -19.935  1.00 25.90      RNA1 C
ATOM  1832  C4*  U C1065      1.022  15.492 -20.286  1.00 32.86      RNA1 C
ATOM  1833  O4*  U C1065      1.493  14.818 -19.094  1.00 35.71      RNA1 O
ATOM  1834  C3*  U C1065      0.721  14.374 -21.270  1.00 35.55      RNA1 C
ATOM  1835  O3*  U C1065      0.799  14.834 -22.609  1.00 37.39      RNA1 O
ATOM  1836  C2*  U C1065      1.793  13.340 -20.939  1.00 36.11      RNA1 C
ATOM  1837  O2*  U C1065      3.047  13.612 -21.536  1.00 27.98      RNA1 O
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ATOM	1838	C1*	U	C1065	1.917	13.505	-19.423	1.00	33.40	RNA1	C
ATOM	1839	N1	U	C1065	1.088	12.543	-18.676	1.00	17.15	RNA1	N
ATOM	1840	C2	U	C1065	1.653	11.323	-18.364	1.00	21.75	RNA1	C
ATOM	1841	O2	U	C1065	2.789	11.015	-18.700	1.00	24.53	RNA1	O
ATOM	1842	N3	U	C1065	0.841	10.472	-17.652	1.00	12.86	RNA1	N
ATOM	1843	C4	U	C1065	-0.454	10.708	-17.245	1.00	22.54	RNA1	C
ATOM	1844	O4	U	C1065	-1.068	9.829	-16.631	1.00	33.30	RNA1	O
ATOM	1845	C5	U	C1065	-0.972	11.988	-17.617	1.00	18.28	RNA1	C
ATOM	1846	C6	U	C1065	-0.202	12.840	-18.300	1.00	12.72	RNA1	C
ATOM	1847	P	U	C1066	-0.290	14.345	-23.688	1.00	38.85	RNA1	P
ATOM	1848	O1P	U	C1066	-1.664	14.499	-23.126	1.00	18.29	RNA1	O
ATOM	1849	O2P	U	C1066	0.064	15.034	-24.964	1.00	40.95	RNA1	O
ATOM	1850	O5*	U	C1066	0.014	12.790	-23.851	1.00	36.40	RNA1	O
ATOM	1851	C5*	U	C1066	1.288	12.346	-24.350	1.00	35.84	RNA1	C
ATOM	1852	C4*	U	C1066	1.461	10.870	-24.107	1.00	38.35	RNA1	C
ATOM	1853	O4*	U	C1066	1.463	10.613	-22.679	1.00	39.66	RNA1	O
ATOM	1854	C3*	U	C1066	0.359	9.974	-24.652	1.00	44.84	RNA1	C
ATOM	1855	O3*	U	C1066	0.570	9.660	-26.021	1.00	45.33	RNA1	O
ATOM	1856	C2*	U	C1066	0.473	8.739	-23.769	1.00	44.55	RNA1	C
ATOM	1857	O2*	U	C1066	1.511	7.884	-24.213	1.00	33.40	RNA1	O
ATOM	1858	C1*	U	C1066	0.859	9.357	-22.421	1.00	39.47	RNA1	C
ATOM	1859	N1	U	C1066	-0.301	9.556	-21.535	1.00	27.32	RNA1	N
ATOM	1860	C2	U	C1066	-0.598	8.548	-20.630	1.00	27.94	RNA1	C
ATOM	1861	O2	U	C1066	0.086	7.545	-20.506	1.00	31.42	RNA1	O
ATOM	1862	N3	U	C1066	-1.722	8.759	-19.869	1.00	19.18	RNA1	N
ATOM	1863	C4	U	C1066	-2.556	9.854	-19.905	1.00	25.49	RNA1	C
ATOM	1864	O4	U	C1066	-3.565	9.870	-19.194	1.00	36.42	RNA1	O
ATOM	1865	C5	U	C1066	-2.168	10.867	-20.840	1.00	19.93	RNA1	C
ATOM	1866	C6	U	C1066	-1.082	10.689	-21.604	1.00	23.45	RNA1	C
ATOM	1867	P	A	C1067	-0.690	9.514	-27.002	1.00	46.85	RNA1	P
ATOM	1868	O1P	A	C1067	-1.666	10.598	-26.712	1.00	36.17	RNA1	O
ATOM	1869	O2P	A	C1067	-0.149	9.350	-28.374	1.00	52.36	RNA1	O
ATOM	1870	O5*	A	C1067	-1.379	8.151	-26.562	1.00	45.01	RNA1	O
ATOM	1871	C5*	A	C1067	-2.763	7.888	-26.874	1.00	42.12	RNA1	C
ATOM	1872	C4*	A	C1067	-3.108	6.464	-26.511	1.00	37.93	RNA1	C
ATOM	1873	O4*	A	C1067	-2.272	5.567	-27.279	1.00	37.30	RNA1	O
ATOM	1874	C3*	A	C1067	-2.805	6.123	-25.068	1.00	39.89	RNA1	C
ATOM	1875	O3*	A	C1067	-3.905	6.462	-24.244	1.00	44.47	RNA1	O
ATOM	1876	C2*	A	C1067	-2.505	4.632	-25.107	1.00	27.28	RNA1	C
ATOM	1877	O2*	A	C1067	-3.664	3.829	-25.084	1.00	44.22	RNA1	O
ATOM	1878	C1*	A	C1067	-1.845	4.494	-26.472	1.00	20.11	RNA1	C
ATOM	1879	N9	A	C1067	-0.389	4.519	-26.443	1.00	16.55	RNA1	N
ATOM	1880	C8	A	C1067	0.450	5.516	-26.872	1.00	13.35	RNA1	C
ATOM	1881	N7	A	C1067	1.722	5.206	-26.785	1.00	21.36	RNA1	N
ATOM	1882	C5	A	C1067	1.715	3.927	-26.244	1.00	6.97	RNA1	C

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ATOM  1883  C6   A C1067     2.746   3.037 -25.917  1.00 18.48      RNA1 C
ATOM  1884  N6   A C1067     4.046   3.301 -26.105  1.00 25.96      RNA1 N
ATOM  1885  N1   A C1067     2.400   1.845 -25.391  1.00 13.59      RNA1 N
ATOM  1886  C2   A C1067     1.102   1.575 -25.214  1.00 28.55      RNA1 C
ATOM  1887  N3   A C1067     0.041   2.326 -25.488  1.00 23.97      RNA1 N
ATOM  1888  C4   A C1067     0.423   3.503 -26.009  1.00 16.34      RNA1 C
ATOM  1889  P    G C1068    -3.632   7.060 -22.783  1.00 39.02      RNA1 P
ATOM  1890  O1P  G C1068    -2.666   8.189 -22.930  1.00 31.97      RNA1 O
ATOM  1891  O2P  G C1068    -4.955   7.282 -22.122  1.00 23.85      RNA1 O
ATOM  1892  O5*  G C1068    -2.872   5.872 -22.052  1.00 29.64      RNA1 O
ATOM  1893  C5*  G C1068    -3.560   4.650 -21.753  1.00 26.14      RNA1 C
ATOM  1894  C4*  G C1068    -2.611   3.675 -21.128  1.00 30.68      RNA1 C
ATOM  1895  O4*  G C1068    -1.612   3.299 -22.105  1.00 33.92      RNA1 O
ATOM  1896  C3*  G C1068    -1.821   4.231 -19.956  1.00 37.79      RNA1 C
ATOM  1897  O3*  G C1068    -2.586   4.140 -18.752  1.00 40.54      RNA1 O
ATOM  1898  C2*  G C1068    -0.564   3.368 -19.963  1.00 31.49      RNA1 C
ATOM  1899  O2*  G C1068    -0.774   2.123 -19.322  1.00 38.55      RNA1 O
ATOM  1900  C1*  G C1068    -0.364   3.120 -21.463  1.00 28.77      RNA1 C
ATOM  1901  N9   G C1068     0.605   3.989 -22.123  1.00 18.63      RNA1 N
ATOM  1902  C8   G C1068     0.381   5.255 -22.612  1.00 21.10      RNA1 C
ATOM  1903  N7   G C1068     1.437   5.779 -23.177  1.00 18.47      RNA1 N
ATOM  1904  C5   G C1068     2.419   4.808 -23.047  1.00 12.57      RNA1 C
ATOM  1905  C6   G C1068     3.776   4.807 -23.476  1.00 23.53      RNA1 C
ATOM  1906  O6   G C1068     4.402   5.696 -24.076  1.00 26.90      RNA1 O
ATOM  1907  N1   G C1068     4.417   3.616 -23.140  1.00 26.41      RNA1 N
ATOM  1908  C2   G C1068     3.831   2.561 -22.479  1.00 23.88      RNA1 C
ATOM  1909  N2   G C1068     4.625   1.500 -22.232  1.00 22.10      RNA1 N
ATOM  1910  N3   G C1068     2.564   2.546 -22.085  1.00 17.30      RNA1 N
ATOM  1911  C4   G C1068     1.924   3.695 -22.396  1.00 15.61      RNA1 C
ATOM  1912  P    A C1069    -2.674   5.408 -17.758  1.00 35.85      RNA1 P
ATOM  1913  O1P  A C1069    -2.982   6.639 -18.536  1.00 34.22      RNA1 O
ATOM  1914  O2P  A C1069    -3.551   5.029 -16.625  1.00 34.69      RNA1 O
ATOM  1915  O5*  A C1069    -1.186   5.532 -17.220  1.00 22.83      RNA1 O
ATOM  1916  C5*  A C1069    -0.570   4.437 -16.545  1.00 16.26      RNA1 C
ATOM  1917  C4*  A C1069     0.859   4.768 -16.237  1.00 21.94      RNA1 C
ATOM  1918  O4*  A C1069     1.694   4.585 -17.417  1.00 35.64      RNA1 O
ATOM  1919  C3*  A C1069     1.093   6.209 -15.768  1.00 37.69      RNA1 C
ATOM  1920  O3*  A C1069     2.058   6.196 -14.714  1.00 40.68      RNA1 O
ATOM  1921  C2*  A C1069     1.737   6.855 -16.996  1.00 39.67      RNA1 C
ATOM  1922  O2*  A C1069     2.583   7.960 -16.731  1.00 43.60      RNA1 O
ATOM  1923  C1*  A C1069     2.567   5.680 -17.491  1.00 37.65      RNA1 C
ATOM  1924  N9   A C1069     3.223   5.772 -18.793  1.00 33.82      RNA1 N
ATOM  1925  C8   A C1069     2.972   6.600 -19.858  1.00 28.66      RNA1 C
ATOM  1926  N7   A C1069     3.878   6.527 -20.805  1.00 37.91      RNA1 N
ATOM  1927  C5   A C1069     4.758   5.554 -20.349  1.00 34.14      RNA1 C
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ATOM	1928	C6	A C1069	5.949	5.022	-20.886	1.00	38.86	RNA1	C
ATOM	1929	N6	A C1069	6.490	5.420	-22.038	1.00	44.62	RNA1	N
ATOM	1930	N1	A C1069	6.577	4.054	-20.180	1.00	40.40	RNA1	N
ATOM	1931	C2	A C1069	6.041	3.661	-19.017	1.00	35.55	RNA1	C
ATOM	1932	N3	A C1069	4.939	4.093	-18.408	1.00	28.51	RNA1	N
ATOM	1933	C4	A C1069	4.342	5.053	-19.133	1.00	31.82	RNA1	C
ATOM	1934	P	A C1070	1.715	6.875	-13.302	1.00	33.11	RNA1	P
ATOM	1935	O1P	A C1070	3.039	7.134	-12.680	1.00	18.08	RNA1	O
ATOM	1936	O2P	A C1070	0.734	7.989	-13.469	1.00	18.52	RNA1	O
ATOM	1937	O5*	A C1070	0.968	5.723	-12.497	1.00	30.46	RNA1	O
ATOM	1938	C5*	A C1070	1.690	4.589	-11.998	1.00	21.05	RNA1	C
ATOM	1939	C4*	A C1070	0.844	3.851	-11.000	1.00	30.01	RNA1	C
ATOM	1940	O4*	A C1070	-0.391	3.424	-11.634	1.00	25.30	RNA1	O
ATOM	1941	C3*	A C1070	1.479	2.612	-10.390	1.00	36.56	RNA1	C
ATOM	1942	O3*	A C1070	1.078	2.564	-9.026	1.00	37.18	RNA1	O
ATOM	1943	C2*	A C1070	0.847	1.469	-11.185	1.00	37.06	RNA1	C
ATOM	1944	O2*	A C1070	0.739	0.256	-10.463	1.00	48.87	RNA1	O
ATOM	1945	C1*	A C1070	-0.539	2.028	-11.495	1.00	32.98	RNA1	C
ATOM	1946	N9	A C1070	-1.107	1.501	-12.735	1.00	42.72	RNA1	N
ATOM	1947	C8	A C1070	-0.659	1.702	-14.019	1.00	49.93	RNA1	C
ATOM	1948	N7	A C1070	-1.380	1.098	-14.929	1.00	50.90	RNA1	N
ATOM	1949	C5	A C1070	-2.366	0.452	-14.198	1.00	55.33	RNA1	C
ATOM	1950	C6	A C1070	-3.435	-0.367	-14.582	1.00	59.78	RNA1	C
ATOM	1951	N6	A C1070	-3.697	-0.683	-15.850	1.00	68.95	RNA1	N
ATOM	1952	N1	A C1070	-4.235	-0.857	-13.608	1.00	56.29	RNA1	N
ATOM	1953	C2	A C1070	-3.965	-0.536	-12.340	1.00	41.79	RNA1	C
ATOM	1954	N3	A C1070	-2.987	0.222	-11.854	1.00	44.24	RNA1	N
ATOM	1955	C4	A C1070	-2.212	0.692	-12.847	1.00	46.56	RNA1	C
ATOM	1956	P	G C1071	2.022	1.866	-7.940	1.00	29.75	RNA1	P
ATOM	1957	O1P	G C1071	1.299	1.985	-6.653	1.00	39.09	RNA1	O
ATOM	1958	O2P	G C1071	2.436	0.526	-8.435	1.00	39.01	RNA1	O
ATOM	1959	O5*	G C1071	3.325	2.769	-7.901	1.00	19.92	RNA1	O
ATOM	1960	C5*	G C1071	3.295	4.113	-7.406	1.00	16.74	RNA1	C
ATOM	1961	C4*	G C1071	4.704	4.562	-7.133	1.00	23.89	RNA1	C
ATOM	1962	O4*	G C1071	5.222	3.769	-6.044	1.00	22.65	RNA1	O
ATOM	1963	C3*	G C1071	5.633	4.285	-8.302	1.00	25.19	RNA1	C
ATOM	1964	O3*	G C1071	5.646	5.390	-9.187	1.00	38.67	RNA1	O
ATOM	1965	C2*	G C1071	6.974	4.006	-7.639	1.00	21.49	RNA1	C
ATOM	1966	O2*	G C1071	7.729	5.164	-7.347	1.00	30.27	RNA1	O
ATOM	1967	C1*	G C1071	6.533	3.335	-6.340	1.00	18.58	RNA1	C
ATOM	1968	N9	G C1071	6.500	1.878	-6.393	1.00	22.64	RNA1	N
ATOM	1969	C8	G C1071	5.389	1.076	-6.272	1.00	20.39	RNA1	C
ATOM	1970	N7	G C1071	5.672	-0.196	-6.315	1.00	31.29	RNA1	N
ATOM	1971	C5	G C1071	7.048	-0.236	-6.482	1.00	14.55	RNA1	C
ATOM	1972	C6	G C1071	7.922	-1.342	-6.582	1.00	28.22	RNA1	C

ATOM	1973	O6	G	C1071	7.647	-2.549	-6.512	1.00	31.85	RNA1 O
ATOM	1974	N1	G	C1071	9.239	-0.934	-6.762	1.00	15.53	RNA1 N
ATOM	1975	C2	G	C1071	9.660	0.371	-6.818	1.00	20.27	RNA1 C
ATOM	1976	N2	G	C1071	10.977	0.567	-6.997	1.00	25.10	RNA1 N
ATOM	1977	N3	G	C1071	8.853	1.411	-6.707	1.00	19.36	RNA1 N
ATOM	1978	C4	G	C1071	7.570	1.035	-6.546	1.00	11.18	RNA1 C
ATOM	1979	P	C	C1072	5.597	5.137	-10.767	1.00	27.21	RNA1 P
ATOM	1980	O1P	C	C1072	4.563	4.110	-11.043	1.00	30.50	RNA1 O
ATOM	1981	O2P	C	C1072	5.512	6.459	-11.426	1.00	25.77	RNA1 O
ATOM	1982	O5*	C	C1072	7.022	4.506	-11.073	1.00	15.96	RNA1 O
ATOM	1983	C5*	C	C1072	8.198	5.315	-11.019	1.00	23.11	RNA1 C
ATOM	1984	C4*	C	C1072	9.419	4.471	-11.280	1.00	32.01	RNA1 C
ATOM	1985	O4*	C	C1072	9.601	3.533	-10.192	1.00	36.03	RNA1 O
ATOM	1986	C3*	C	C1072	9.365	3.597	-12.522	1.00	30.99	RNA1 C
ATOM	1987	O3*	C	C1072	9.711	4.326	-13.688	1.00	33.23	RNA1 O
ATOM	1988	C2*	C	C1072	10.362	2.496	-12.188	1.00	29.75	RNA1 C
ATOM	1989	O2*	C	C1072	11.703	2.904	-12.371	1.00	34.64	RNA1 O
ATOM	1990	C1*	C	C1072	10.121	2.314	-10.692	1.00	29.06	RNA1 C
ATOM	1991	N1	C	C1072	9.151	1.242	-10.401	1.00	21.88	RNA1 N
ATOM	1992	C2	C	C1072	9.623	-0.062	-10.229	1.00	22.42	RNA1 C
ATOM	1993	O2	C	C1072	10.852	-0.281	-10.328	1.00	27.87	RNA1 O
ATOM	1994	N3	C	C1072	8.735	-1.053	-9.964	1.00	9.91	RNA1 N
ATOM	1995	C4	C	C1072	7.430	-0.780	-9.883	1.00	19.29	RNA1 C
ATOM	1996	N4	C	C1072	6.591	-1.789	-9.644	1.00	23.91	RNA1 N
ATOM	1997	C5	C	C1072	6.925	0.538	-10.048	1.00	13.70	RNA1 C
ATOM	1998	C6	C	C1072	7.812	1.510	-10.304	1.00	24.95	RNA1 C
ATOM	1999	P	A	C1073	8.702	4.336	-14.936	1.00	33.99	RNA1 P
ATOM	2000	O1P	A	C1073	8.504	2.919	-15.333	1.00	35.83	RNA1 O
ATOM	2001	O2P	A	C1073	7.512	5.181	-14.614	1.00	22.96	RNA1 O
ATOM	2002	O5*	A	C1073	9.551	5.050	-16.074	1.00	31.36	RNA1 O
ATOM	2003	C5*	A	C1073	10.772	4.462	-16.571	1.00	35.37	RNA1 C
ATOM	2004	C4*	A	C1073	11.245	5.227	-17.781	1.00	39.45	RNA1 C
ATOM	2005	O4*	A	C1073	10.229	5.143	-18.815	1.00	39.78	RNA1 O
ATOM	2006	C3*	A	C1073	11.400	6.713	-17.522	1.00	40.87	RNA1 C
ATOM	2007	O3*	A	C1073	12.673	7.017	-16.987	1.00	44.46	RNA1 O
ATOM	2008	C2*	A	C1073	11.147	7.327	-18.890	1.00	38.57	RNA1 C
ATOM	2009	O2*	A	C1073	12.279	7.252	-19.738	1.00	41.89	RNA1 O
ATOM	2010	C1*	A	C1073	10.054	6.409	-19.426	1.00	27.18	RNA1 C
ATOM	2011	N9	A	C1073	8.713	6.872	-19.081	1.00	23.78	RNA1 N
ATOM	2012	C8	A	C1073	7.835	6.282	-18.209	1.00	31.10	RNA1 C
ATOM	2013	N7	A	C1073	6.685	6.903	-18.112	1.00	30.54	RNA1 N
ATOM	2014	C5	A	C1073	6.819	7.979	-18.974	1.00	22.89	RNA1 C
ATOM	2015	C6	A	C1073	5.948	9.015	-19.319	1.00	24.05	RNA1 C
ATOM	2016	N6	A	C1073	4.711	9.130	-18.836	1.00	24.67	RNA1 N
ATOM	2017	N1	A	C1073	6.391	9.940	-20.193	1.00	27.06	RNA1 N

ATOM	2018	C2	A	C1073	7.627	9.815	-20.684	1.00	28.92	RNA1	C
ATOM	2019	N3	A	C1073	8.539	8.879	-20.442	1.00	33.22	RNA1	N
ATOM	2020	C4	A	C1073	8.066	7.979	-19.568	1.00	24.70	RNA1	C
ATOM	2021	P	G	C1074	12.790	8.131	-15.846	1.00	37.49	RNA1	P
ATOM	2022	O1P	G	C1074	11.994	7.638	-14.698	1.00	42.76	RNA1	O
ATOM	2023	O2P	G	C1074	14.226	8.458	-15.661	1.00	37.27	RNA1	O
ATOM	2024	O5*	G	C1074	12.052	9.389	-16.488	1.00	32.12	RNA1	O
ATOM	2025	C5*	G	C1074	12.636	10.074	-17.611	1.00	30.38	RNA1	C
ATOM	2026	C4*	G	C1074	11.776	11.239	-18.042	1.00	29.26	RNA1	C
ATOM	2027	O4*	G	C1074	10.505	10.762	-18.552	1.00	28.39	RNA1	O
ATOM	2028	C3*	G	C1074	11.393	12.245	-16.972	1.00	30.49	RNA1	C
ATOM	2029	O3*	G	C1074	12.431	13.170	-16.697	1.00	40.29	RNA1	O
ATOM	2030	C2*	G	C1074	10.152	12.899	-17.566	1.00	32.10	RNA1	C
ATOM	2031	O2*	G	C1074	10.452	13.891	-18.528	1.00	36.08	RNA1	O
ATOM	2032	C1*	G	C1074	9.491	11.714	-18.268	1.00	26.45	RNA1	C
ATOM	2033	N9	G	C1074	8.479	11.075	-17.435	1.00	22.10	RNA1	N
ATOM	2034	C8	G	C1074	8.576	9.862	-16.794	1.00	21.18	RNA1	C
ATOM	2035	N7	G	C1074	7.490	9.539	-16.145	1.00	28.77	RNA1	N
ATOM	2036	C5	G	C1074	6.628	10.604	-16.362	1.00	15.54	RNA1	C
ATOM	2037	C6	G	C1074	5.300	10.815	-15.917	1.00	22.89	RNA1	C
ATOM	2038	O6	G	C1074	4.589	10.071	-15.240	1.00	28.81	RNA1	O
ATOM	2039	N1	G	C1074	4.802	12.038	-16.351	1.00	26.73	RNA1	N
ATOM	2040	C2	G	C1074	5.487	12.937	-17.126	1.00	24.75	RNA1	C
ATOM	2041	N2	G	C1074	4.828	14.058	-17.440	1.00	20.91	RNA1	N
ATOM	2042	N3	G	C1074	6.724	12.748	-17.560	1.00	19.40	RNA1	N
ATOM	2043	C4	G	C1074	7.228	11.568	-17.144	1.00	19.49	RNA1	C
ATOM	2044	P	C	C1075	12.535	13.826	-15.232	1.00	35.74	RNA1	P
ATOM	2045	O1P	C	C1075	12.251	12.757	-14.239	1.00	37.48	RNA1	O
ATOM	2046	O2P	C	C1075	13.814	14.574	-15.147	1.00	35.45	RNA1	O
ATOM	2047	O5*	C	C1075	11.326	14.864	-15.223	1.00	29.10	RNA1	O
ATOM	2048	C5*	C	C1075	11.373	16.035	-16.052	1.00	20.72	RNA1	C
ATOM	2049	C4*	C	C1075	10.144	16.884	-15.848	1.00	27.73	RNA1	C
ATOM	2050	O4*	C	C1075	8.980	16.162	-16.316	1.00	25.49	RNA1	O
ATOM	2051	C3*	C	C1075	9.804	17.254	-14.413	1.00	29.84	RNA1	C
ATOM	2052	O3*	C	C1075	10.548	18.355	-13.924	1.00	32.76	RNA1	O
ATOM	2053	C2*	C	C1075	8.311	17.537	-14.490	1.00	32.29	RNA1	C
ATOM	2054	O2*	C	C1075	8.018	18.838	-14.963	1.00	33.04	RNA1	O
ATOM	2055	C1*	C	C1075	7.860	16.488	-15.508	1.00	30.74	RNA1	C
ATOM	2056	N1	C	C1075	7.407	15.259	-14.836	1.00	23.00	RNA1	N
ATOM	2057	C2	C	C1075	6.083	15.178	-14.407	1.00	25.39	RNA1	C
ATOM	2058	O2	C	C1075	5.320	16.133	-14.627	1.00	27.71	RNA1	O
ATOM	2059	N3	C	C1075	5.666	14.063	-13.764	1.00	20.56	RNA1	N
ATOM	2060	C4	C	C1075	6.518	13.054	-13.553	1.00	24.69	RNA1	C
ATOM	2061	N4	C	C1075	6.067	11.975	-12.911	1.00	22.56	RNA1	N
ATOM	2062	C5	C	C1075	7.870	13.108	-13.991	1.00	16.20	RNA1	C

ATOM	2063	C6	C	C1075	8.269	14.217	-14.622	1.00	23.77	RNA1	C
ATOM	2064	P	C	C1076	10.912	18.423	-12.358	1.00	42.91	RNA1	P
ATOM	2065	O1P	C	C1076	11.372	17.085	-11.911	1.00	24.52	RNA1	O
ATOM	2066	O2P	C	C1076	11.781	19.612	-12.113	1.00	41.73	RNA1	O
ATOM	2067	O5*	C	C1076	9.491	18.679	-11.696	1.00	32.86	RNA1	O
ATOM	2068	C5*	C	C1076	8.768	19.870	-11.997	1.00	27.46	RNA1	C
ATOM	2069	C4*	C	C1076	7.458	19.893	-11.255	1.00	30.86	RNA1	C
ATOM	2070	O4*	C	C1076	6.570	18.885	-11.798	1.00	34.77	RNA1	O
ATOM	2071	C3*	C	C1076	7.500	19.581	-9.769	1.00	26.66	RNA1	C
ATOM	2072	O3*	C	C1076	7.913	20.668	-8.961	1.00	36.57	RNA1	O
ATOM	2073	C2*	C	C1076	6.062	19.172	-9.499	1.00	32.47	RNA1	C
ATOM	2074	O2*	C	C1076	5.198	20.290	-9.410	1.00	32.97	RNA1	O
ATOM	2075	C1*	C	C1076	5.735	18.385	-10.765	1.00	34.29	RNA1	C
ATOM	2076	N1	C	C1076	6.012	16.945	-10.577	1.00	22.34	RNA1	N
ATOM	2077	C2	C	C1076	5.036	16.150	-9.959	1.00	24.18	RNA1	C
ATOM	2078	O2	C	C1076	3.977	16.680	-9.577	1.00	25.15	RNA1	O
ATOM	2079	N3	C	C1076	5.271	14.825	-9.784	1.00	20.85	RNA1	N
ATOM	2080	C4	C	C1076	6.428	14.295	-10.185	1.00	21.45	RNA1	C
ATOM	2081	N4	C	C1076	6.611	12.987	-9.994	1.00	19.48	RNA1	N
ATOM	2082	C5	C	C1076	7.446	15.083	-10.805	1.00	18.25	RNA1	C
ATOM	2083	C6	C	C1076	7.196	16.389	-10.984	1.00	25.90	RNA1	C
ATOM	2084	P	A	C1077	8.725	20.374	-7.602	1.00	34.53	RNA1	P
ATOM	2085	O1P	A	C1077	9.776	19.366	-7.891	1.00	32.29	RNA1	O
ATOM	2086	O2P	A	C1077	9.115	21.689	-7.025	1.00	55.02	RNA1	O
ATOM	2087	O5*	A	C1077	7.641	19.691	-6.652	1.00	22.72	RNA1	O
ATOM	2088	C5*	A	C1077	6.447	20.399	-6.283	1.00	17.11	RNA1	C
ATOM	2089	C4*	A	C1077	5.461	19.477	-5.601	1.00	26.56	RNA1	C
ATOM	2090	O4*	A	C1077	5.058	18.423	-6.514	1.00	34.54	RNA1	O
ATOM	2091	C3*	A	C1077	5.916	18.724	-4.357	1.00	32.85	RNA1	C
ATOM	2092	O3*	A	C1077	5.872	19.511	-3.175	1.00	37.36	RNA1	O
ATOM	2093	C2*	A	C1077	4.913	17.576	-4.297	1.00	36.94	RNA1	C
ATOM	2094	O2*	A	C1077	3.661	17.943	-3.748	1.00	32.73	RNA1	O
ATOM	2095	C1*	A	C1077	4.723	17.255	-5.778	1.00	32.51	RNA1	C
ATOM	2096	N9	A	C1077	5.612	16.160	-6.172	1.00	27.14	RNA1	N
ATOM	2097	C8	A	C1077	6.830	16.224	-6.802	1.00	22.59	RNA1	C
ATOM	2098	N7	A	C1077	7.406	15.054	-6.959	1.00	28.95	RNA1	N
ATOM	2099	C5	A	C1077	6.500	14.158	-6.405	1.00	23.18	RNA1	C
ATOM	2100	C6	A	C1077	6.524	12.758	-6.252	1.00	29.03	RNA1	C
ATOM	2101	N6	A	C1077	7.543	11.984	-6.643	1.00	32.89	RNA1	N
ATOM	2102	N1	A	C1077	5.454	12.174	-5.669	1.00	23.42	RNA1	N
ATOM	2103	C2	A	C1077	4.443	12.948	-5.259	1.00	10.65	RNA1	C
ATOM	2104	N3	A	C1077	4.309	14.266	-5.338	1.00	26.74	RNA1	N
ATOM	2105	C4	A	C1077	5.385	14.821	-5.930	1.00	26.08	RNA1	C
ATOM	2106	P	U	C1078	6.978	19.284	-2.026	1.00	29.17	RNA1	P
ATOM	2107	O1P	U	C1078	8.330	19.420	-2.616	1.00	22.94	RNA1	O

ATOM	2108	O2P	U	C1078	6.586	20.141	-0.877	1.00	41.57	RNA1	O
ATOM	2109	O5*	U	C1078	6.828	17.754	-1.608	1.00	29.90	RNA1	O
ATOM	2110	C5*	U	C1078	5.706	17.287	-0.830	1.00	21.78	RNA1	C
ATOM	2111	C4*	U	C1078	5.789	15.785	-0.649	1.00	21.19	RNA1	C
ATOM	2112	O4*	U	C1078	5.732	15.157	-1.957	1.00	29.99	RNA1	O
ATOM	2113	C3*	U	C1078	7.075	15.241	-0.031	1.00	27.77	RNA1	C
ATOM	2114	O3*	U	C1078	7.057	15.184	1.390	1.00	36.77	RNA1	O
ATOM	2115	C2*	U	C1078	7.094	13.812	-0.554	1.00	34.85	RNA1	C
ATOM	2116	O2*	U	C1078	6.229	12.972	0.191	1.00	32.65	RNA1	O
ATOM	2117	C1*	U	C1078	6.532	13.986	-1.963	1.00	28.35	RNA1	C
ATOM	2118	N1	U	C1078	7.611	14.137	-2.955	1.00	21.70	RNA1	N
ATOM	2119	C2	U	C1078	8.275	12.987	-3.352	1.00	27.00	RNA1	C
ATOM	2120	O2	U	C1078	7.975	11.872	-2.946	1.00	29.58	RNA1	O
ATOM	2121	N3	U	C1078	9.305	13.189	-4.238	1.00	24.66	RNA1	N
ATOM	2122	C4	U	C1078	9.728	14.393	-4.760	1.00	26.71	RNA1	C
ATOM	2123	O4	U	C1078	10.714	14.417	-5.504	1.00	44.05	RNA1	O
ATOM	2124	C5	U	C1078	8.978	15.530	-4.320	1.00	18.54	RNA1	C
ATOM	2125	C6	U	C1078	7.970	15.368	-3.459	1.00	19.12	RNA1	C
ATOM	2126	P	C	C1079	7.168	16.527	2.260	1.00	28.61	RNA1	P
ATOM	2127	O1P	C	C1079	7.780	16.107	3.544	1.00	34.30	RNA1	O
ATOM	2128	O2P	C	C1079	7.770	17.644	1.487	1.00	31.33	RNA1	O
ATOM	2129	O5*	C	C1079	5.641	16.867	2.520	1.00	13.04	RNA1	O
ATOM	2130	C5*	C	C1079	4.851	15.965	3.271	1.00	17.43	RNA1	C
ATOM	2131	C4*	C	C1079	3.398	16.246	3.064	1.00	19.74	RNA1	C
ATOM	2132	O4*	C	C1079	2.954	15.688	1.803	1.00	26.36	RNA1	O
ATOM	2133	C3*	C	C1079	2.556	15.540	4.098	1.00	25.66	RNA1	C
ATOM	2134	O3*	C	C1079	2.525	16.312	5.278	1.00	37.56	RNA1	O
ATOM	2135	C2*	C	C1079	1.217	15.382	3.394	1.00	27.27	RNA1	C
ATOM	2136	O2*	C	C1079	0.452	16.573	3.416	1.00	25.00	RNA1	O
ATOM	2137	C1*	C	C1079	1.672	15.091	1.963	1.00	17.88	RNA1	C
ATOM	2138	N1	C	C1079	1.795	13.641	1.677	1.00	17.52	RNA1	N
ATOM	2139	C2	C	C1079	0.629	12.878	1.441	1.00	19.34	RNA1	C
ATOM	2140	O2	C	C1079	-0.488	13.427	1.500	1.00	24.52	RNA1	O
ATOM	2141	N3	C	C1079	0.748	11.561	1.159	1.00	15.18	RNA1	N
ATOM	2142	C4	C	C1079	1.955	10.994	1.111	1.00	20.12	RNA1	C
ATOM	2143	N4	C	C1079	2.018	9.691	0.814	1.00	14.62	RNA1	N
ATOM	2144	C5	C	C1079	3.150	11.734	1.359	1.00	16.35	RNA1	C
ATOM	2145	C6	C	C1079	3.025	13.040	1.635	1.00	14.99	RNA1	C
ATOM	2146	P	A	C1080	2.747	15.593	6.692	1.00	32.18	RNA1	P
ATOM	2147	O1P	A	C1080	3.901	14.668	6.598	1.00	27.65	RNA1	O
ATOM	2148	O2P	A	C1080	2.748	16.674	7.711	1.00	42.21	RNA1	O
ATOM	2149	O5*	A	C1080	1.413	14.745	6.853	1.00	24.30	RNA1	O
ATOM	2150	C5*	A	C1080	0.157	15.421	6.836	1.00	25.92	RNA1	C
ATOM	2151	C4*	A	C1080	-0.967	14.459	6.593	1.00	27.37	RNA1	C
ATOM	2152	O4*	A	C1080	-0.902	13.924	5.248	1.00	35.15	RNA1	O

ATOM	2153	C3*	A	C1080	-1.028	13.223	7.462	1.00	26.09	RNA1 C
ATOM	2154	O3*	A	C1080	-1.528	13.489	8.759	1.00	36.10	RNA1 O
ATOM	2155	C2*	A	C1080	-1.956	12.331	6.651	1.00	33.11	RNA1 C
ATOM	2156	O2*	A	C1080	-3.309	12.717	6.787	1.00	32.80	RNA1 O
ATOM	2157	C1*	A	C1080	-1.510	12.643	5.223	1.00	26.83	RNA1 C
ATOM	2158	N9	A	C1080	-0.538	11.650	4.767	1.00	16.76	RNA1 N
ATOM	2159	C8	A	C1080	0.838	11.722	4.719	1.00	20.21	RNA1 C
ATOM	2160	N7	A	C1080	1.411	10.609	4.319	1.00	8.53	RNA1 N
ATOM	2161	C5	A	C1080	0.340	9.754	4.073	1.00	7.38	RNA1 C
ATOM	2162	C6	A	C1080	0.273	8.414	3.649	1.00	15.76	RNA1 C
ATOM	2163	N6	A	C1080	1.348	7.660	3.376	1.00	25.46	RNA1 N
ATOM	2164	N1	A	C1080	-0.952	7.859	3.514	1.00	17.62	RNA1 N
ATOM	2165	C2	A	C1080	-2.029	8.606	3.785	1.00	16.21	RNA1 C
ATOM	2166	N3	A	C1080	-2.095	9.868	4.192	1.00	17.28	RNA1 N
ATOM	2167	C4	A	C1080	-0.861	10.389	4.323	1.00	7.47	RNA1 C
ATOM	2168	P	U	C1081	-1.136	12.505	9.973	1.00	29.01	RNA1 P
ATOM	2169	O1P	U	C1081	0.273	12.088	9.807	1.00	19.32	RNA1 O
ATOM	2170	O2P	U	C1081	-1.558	13.151	11.237	1.00	36.17	RNA1 O
ATOM	2171	O5*	U	C1081	-2.072	11.248	9.708	1.00	27.53	RNA1 O
ATOM	2172	C5*	U	C1081	-3.469	11.439	9.421	1.00	34.97	RNA1 C
ATOM	2173	C4*	U	C1081	-4.093	10.146	8.967	1.00	39.34	RNA1 C
ATOM	2174	O4*	U	C1081	-3.488	9.719	7.725	1.00	36.64	RNA1 O
ATOM	2175	C3*	U	C1081	-3.908	8.982	9.922	1.00	36.77	RNA1 C
ATOM	2176	O3*	U	C1081	-4.954	9.001	10.888	1.00	49.64	RNA1 O
ATOM	2177	C2*	U	C1081	-4.001	7.774	9.001	1.00	31.27	RNA1 C
ATOM	2178	O2*	U	C1081	-5.344	7.418	8.739	1.00	35.76	RNA1 O
ATOM	2179	C1*	U	C1081	-3.375	8.311	7.713	1.00	27.99	RNA1 C
ATOM	2180	N1	U	C1081	-1.959	7.966	7.513	1.00	16.45	RNA1 N
ATOM	2181	C2	U	C1081	-1.659	6.684	7.082	1.00	15.53	RNA1 C
ATOM	2182	O2	U	C1081	-2.511	5.822	6.912	1.00	24.70	RNA1 O
ATOM	2183	N3	U	C1081	-0.328	6.446	6.856	1.00	6.42	RNA1 N
ATOM	2184	C4	U	C1081	0.717	7.335	7.015	1.00	17.75	RNA1 C
ATOM	2185	O4	U	C1081	1.850	7.005	6.656	1.00	12.74	RNA1 O
ATOM	2186	C5	U	C1081	0.332	8.627	7.495	1.00	15.50	RNA1 C
ATOM	2187	C6	U	C1081	-0.961	8.890	7.724	1.00	17.69	RNA1 C
ATOM	2188	P	U	C1082	-4.709	8.375	12.348	1.00	43.16	RNA1 P
ATOM	2189	O1P	U	C1082	-3.513	9.034	12.942	1.00	33.87	RNA1 O
ATOM	2190	O2P	U	C1082	-6.019	8.423	13.060	1.00	35.46	RNA1 O
ATOM	2191	O5*	U	C1082	-4.357	6.855	12.050	1.00	39.66	RNA1 O
ATOM	2192	C5*	U	C1082	-5.388	5.949	11.643	1.00	36.85	RNA1 C
ATOM	2193	C4*	U	C1082	-4.834	4.563	11.500	1.00	35.35	RNA1 C
ATOM	2194	O4*	U	C1082	-4.024	4.471	10.301	1.00	27.83	RNA1 O
ATOM	2195	C3*	U	C1082	-3.895	4.106	12.600	1.00	42.67	RNA1 C
ATOM	2196	O3*	U	C1082	-4.544	3.677	13.786	1.00	48.43	RNA1 O
ATOM	2197	C2*	U	C1082	-3.130	2.979	11.925	1.00	41.00	RNA1 C

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ATOM  2198 O2*  U C1082    -3.847  1.757 11.941 1.00 43.11    RNA1 O
ATOM  2199 C1*  U C1082    -3.000  3.510 10.496 1.00 29.73    RNA1 C
ATOM  2200 N1   U C1082    -1.691  4.146 10.281 1.00 21.48    RNA1 N
ATOM  2201 C2   U C1082    -0.650  3.342  9.826 1.00 24.74    RNA1 C
ATOM  2202 O2   U C1082    -0.781  2.155  9.573 1.00 35.44    RNA1 O
ATOM  2203 N3   U C1082     0.552  3.980  9.678 1.00 16.73    RNA1 N
ATOM  2204 C4   U C1082     0.825  5.303  9.921 1.00 20.16    RNA1 C
ATOM  2205 O4   U C1082     1.963  5.730  9.715 1.00 29.48    RNA1 O
ATOM  2206 C5   U C1082    -0.293  6.069 10.378 1.00 15.77    RNA1 C
ATOM  2207 C6   U C1082    -1.485  5.479 10.536 1.00 20.32    RNA1 C
ATOM  2208 P    U C1083    -3.685  3.548 15.138 1.00 44.11    RNA1 P
ATOM  2209 O1P  U C1083    -3.013  4.855 15.416 1.00 33.72    RNA1 O
ATOM  2210 O2P  U C1083    -4.550  2.923 16.170 1.00 44.56    RNA1 O
ATOM  2211 O5*  U C1083    -2.554  2.515 14.732 1.00 26.53    RNA1 O
ATOM  2212 C5*  U C1083    -1.204  2.710 15.133 1.00 27.01    RNA1 C
ATOM  2213 C4*  U C1083    -0.310  1.810 14.328 1.00 35.50    RNA1 C
ATOM  2214 O4*  U C1083     0.049  2.450 13.077 1.00 37.83    RNA1 O
ATOM  2215 C3*  U C1083     1.014  1.490 14.985 1.00 42.54    RNA1 C
ATOM  2216 O3*  U C1083     0.829  0.394 15.868 1.00 53.77    RNA1 O
ATOM  2217 C2*  U C1083     1.899  1.142 13.797 1.00 40.40    RNA1 C
ATOM  2218 O2*  U C1083     1.676 -0.184 13.354 1.00 50.14    RNA1 O
ATOM  2219 C1*  U C1083     1.383  2.112 12.733 1.00 31.81    RNA1 C
ATOM  2220 N1   U C1083     2.176  3.350 12.641 1.00 27.07    RNA1 N
ATOM  2221 C2   U C1083     3.403  3.291 11.995 1.00 27.98    RNA1 C
ATOM  2222 O2   U C1083     3.842  2.278 11.491 1.00 38.26    RNA1 O
ATOM  2223 N3   U C1083     4.101  4.471 11.959 1.00 27.06    RNA1 N
ATOM  2224 C4   U C1083     3.711  5.686 12.480 1.00 29.89    RNA1 C
ATOM  2225 O4   U C1083     4.463  6.660 12.376 1.00 35.97    RNA1 O
ATOM  2226 C5   U C1083     2.432  5.676 13.120 1.00 28.35    RNA1 C
ATOM  2227 C6   U C1083     1.726  4.538 13.180 1.00 34.18    RNA1 C
ATOM  2228 P    A C1084     1.531  0.409 17.308 1.00 46.22    RNA1 P
ATOM  2229 O1P  A C1084     1.502  1.811 17.819 1.00 47.82    RNA1 O
ATOM  2230 O2P  A C1084     0.915 -0.683 18.102 1.00 45.99    RNA1 O
ATOM  2231 O5*  A C1084     3.037  0.024 16.984 1.00 32.44    RNA1 O
ATOM  2232 C5*  A C1084     4.103  0.403 17.854 1.00 26.01    RNA1 C
ATOM  2233 C4*  A C1084     5.395 -0.104 17.293 1.00 30.31    RNA1 C
ATOM  2234 O4*  A C1084     5.314 -1.544 17.185 1.00 39.98    RNA1 O
ATOM  2235 C3*  A C1084     5.631  0.378 15.881 1.00 31.04    RNA1 C
ATOM  2236 O3*  A C1084     6.308  1.611 15.926 1.00 35.76    RNA1 O
ATOM  2237 C2*  A C1084     6.448 -0.741 15.252 1.00 34.39    RNA1 C
ATOM  2238 O2*  A C1084     7.825 -0.635 15.548 1.00 29.53    RNA1 O
ATOM  2239 C1*  A C1084     5.872 -1.970 15.956 1.00 36.40    RNA1 C
ATOM  2240 N9   A C1084     4.827 -2.698 15.230 1.00 38.88    RNA1 N
ATOM  2241 C8   A C1084     3.464 -2.577 15.388 1.00 38.21    RNA1 C
ATOM  2242 N7   A C1084     2.770 -3.432 14.677 1.00 33.92    RNA1 N
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ATOM	2243	C5	A	C1084	3.737	-4.151	13.984	1.00	35.92	RNA1	C
ATOM	2244	C6	A	C1084	3.648	-5.222	13.069	1.00	34.35	RNA1	C
ATOM	2245	N6	A	C1084	2.493	-5.781	12.695	1.00	38.02	RNA1	N
ATOM	2246	N1	A	C1084	4.802	-5.704	12.551	1.00	36.24	RNA1	N
ATOM	2247	C2	A	C1084	5.960	-5.145	12.935	1.00	38.72	RNA1	C
ATOM	2248	N3	A	C1084	6.173	-4.143	13.790	1.00	34.15	RNA1	N
ATOM	2249	C4	A	C1084	5.007	-3.689	14.291	1.00	36.93	RNA1	C
ATOM	2250	P	A	C1085	5.839	2.793	14.965	1.00	32.91	RNA1	P
ATOM	2251	O1P	A	C1085	4.351	2.768	14.939	1.00	23.95	RNA1	O
ATOM	2252	O2P	A	C1085	6.554	4.030	15.366	1.00	36.15	RNA1	O
ATOM	2253	O5*	A	C1085	6.414	2.342	13.557	1.00	34.02	RNA1	O
ATOM	2254	C5*	A	C1085	7.826	2.172	13.384	1.00	35.68	RNA1	C
ATOM	2255	C4*	A	C1085	8.100	1.383	12.136	1.00	40.49	RNA1	C
ATOM	2256	O4*	A	C1085	7.592	0.035	12.283	1.00	46.64	RNA1	O
ATOM	2257	C3*	A	C1085	7.426	1.921	10.889	1.00	37.28	RNA1	C
ATOM	2258	O3*	A	C1085	8.249	2.933	10.322	1.00	38.08	RNA1	O
ATOM	2259	C2*	A	C1085	7.311	0.685	10.002	1.00	36.45	RNA1	C
ATOM	2260	O2*	A	C1085	8.496	0.425	9.278	1.00	44.66	RNA1	O
ATOM	2261	C1*	A	C1085	7.122	-0.432	11.032	1.00	36.77	RNA1	C
ATOM	2262	N9	A	C1085	5.743	-0.875	11.198	1.00	24.80	RNA1	N
ATOM	2263	C8	A	C1085	4.754	-0.265	11.923	1.00	28.92	RNA1	C
ATOM	2264	N7	A	C1085	3.606	-0.896	11.888	1.00	28.93	RNA1	N
ATOM	2265	C5	A	C1085	3.857	-2.000	11.087	1.00	22.34	RNA1	C
ATOM	2266	C6	A	C1085	3.040	-3.060	10.664	1.00	26.52	RNA1	C
ATOM	2267	N6	A	C1085	1.749	-3.175	11.000	1.00	26.24	RNA1	N
ATOM	2268	N1	A	C1085	3.596	-4.006	9.874	1.00	25.01	RNA1	N
ATOM	2269	C2	A	C1085	4.889	-3.875	9.532	1.00	27.90	RNA1	C
ATOM	2270	N3	A	C1085	5.758	-2.920	9.864	1.00	23.94	RNA1	N
ATOM	2271	C4	A	C1085	5.171	-2.002	10.654	1.00	23.81	RNA1	C
ATOM	2272	P	A	C1086	7.578	4.220	9.636	1.00	38.44	RNA1	P
ATOM	2273	O1P	A	C1086	6.238	4.440	10.244	1.00	21.00	RNA1	O
ATOM	2274	O2P	A	C1086	8.578	5.315	9.641	1.00	32.04	RNA1	O
ATOM	2275	O5*	A	C1086	7.359	3.750	8.133	1.00	44.64	RNA1	O
ATOM	2276	C5*	A	C1086	8.465	3.286	7.337	1.00	27.97	RNA1	C
ATOM	2277	C4*	A	C1086	7.965	2.407	6.217	1.00	34.03	RNA1	C
ATOM	2278	O4*	A	C1086	7.509	1.138	6.753	1.00	34.69	RNA1	O
ATOM	2279	C3*	A	C1086	6.759	2.929	5.455	1.00	38.31	RNA1	C
ATOM	2280	O3*	A	C1086	7.095	3.913	4.484	1.00	30.65	RNA1	O
ATOM	2281	C2*	A	C1086	6.166	1.659	4.850	1.00	40.89	RNA1	C
ATOM	2282	O2*	A	C1086	6.734	1.284	3.610	1.00	37.38	RNA1	O
ATOM	2283	C1*	A	C1086	6.488	0.616	5.925	1.00	29.88	RNA1	C
ATOM	2284	N9	A	C1086	5.326	0.253	6.739	1.00	26.28	RNA1	N
ATOM	2285	C8	A	C1086	4.885	-1.015	7.018	1.00	26.71	RNA1	C
ATOM	2286	N7	A	C1086	3.748	-1.049	7.675	1.00	32.50	RNA1	N
ATOM	2287	C5	A	C1086	3.437	0.289	7.869	1.00	23.83	RNA1	C

ATOM	2288	C6	A	C1086	2.346	0.926	8.486	1.00	32.24	RNA1	C
ATOM	2289	N6	A	C1086	1.320	0.274	9.042	1.00	40.46	RNA1	N
ATOM	2290	N1	A	C1086	2.340	2.275	8.508	1.00	27.06	RNA1	N
ATOM	2291	C2	A	C1086	3.359	2.928	7.943	1.00	26.31	RNA1	C
ATOM	2292	N3	A	C1086	4.435	2.444	7.329	1.00	27.72	RNA1	N
ATOM	2293	C4	A	C1086	4.413	1.102	7.323	1.00	23.09	RNA1	C
ATOM	2294	P	G	C1087	6.254	5.281	4.430	1.00	30.97	RNA1	P
ATOM	2295	O1P	G	C1087	4.896	4.969	3.921	1.00	19.34	RNA1	O
ATOM	2296	O2P	G	C1087	6.402	5.980	5.734	1.00	46.09	RNA1	O
ATOM	2297	O5*	G	C1087	7.006	6.141	3.329	1.00	29.62	RNA1	O
ATOM	2298	C5*	G	C1087	8.108	6.998	3.667	1.00	28.45	RNA1	C
ATOM	2299	C4*	G	C1087	8.911	7.283	2.428	1.00	31.27	RNA1	C
ATOM	2300	O4*	G	C1087	9.604	6.075	2.060	1.00	35.33	RNA1	O
ATOM	2301	C3*	G	C1087	8.034	7.656	1.244	1.00	31.37	RNA1	C
ATOM	2302	O3*	G	C1087	7.978	9.077	1.163	1.00	19.46	RNA1	O
ATOM	2303	C2*	G	C1087	8.776	7.064	0.049	1.00	32.80	RNA1	C
ATOM	2304	O2*	G	C1087	9.745	7.961	-0.462	1.00	29.59	RNA1	O
ATOM	2305	C1*	G	C1087	9.484	5.854	0.674	1.00	27.32	RNA1	C
ATOM	2306	N9	G	C1087	8.899	4.525	0.520	1.00	19.62	RNA1	N
ATOM	2307	C8	G	C1087	7.596	4.129	0.735	1.00	23.90	RNA1	C
ATOM	2308	N7	G	C1087	7.429	2.836	0.618	1.00	9.45	RNA1	N
ATOM	2309	C5	G	C1087	8.685	2.359	0.273	1.00	16.55	RNA1	C
ATOM	2310	C6	G	C1087	9.128	1.036	0.007	1.00	25.58	RNA1	C
ATOM	2311	O6	G	C1087	8.476	-0.016	0.029	1.00	25.76	RNA1	O
ATOM	2312	N1	G	C1087	10.483	1.004	-0.307	1.00	13.38	RNA1	N
ATOM	2313	C2	G	C1087	11.309	2.103	-0.354	1.00	25.58	RNA1	C
ATOM	2314	N2	G	C1087	12.595	1.870	-0.653	1.00	21.09	RNA1	N
ATOM	2315	N3	G	C1087	10.906	3.341	-0.116	1.00	22.18	RNA1	N
ATOM	2316	C4	G	C1087	9.596	3.394	0.191	1.00	16.33	RNA1	C
ATOM	2317	P	A	C1088	6.677	9.862	1.669	1.00	23.48	RNA1	P
ATOM	2318	O1P	A	C1088	6.035	9.121	2.788	1.00	34.67	RNA1	O
ATOM	2319	O2P	A	C1088	7.106	11.267	1.858	1.00	30.75	RNA1	O
ATOM	2320	O5*	A	C1088	5.683	9.810	0.434	1.00	34.79	RNA1	O
ATOM	2321	C5*	A	C1088	6.166	10.084	-0.886	1.00	33.74	RNA1	C
ATOM	2322	C4*	A	C1088	5.808	8.952	-1.804	1.00	29.37	RNA1	C
ATOM	2323	O4*	A	C1088	4.376	8.744	-1.752	1.00	30.18	RNA1	O
ATOM	2324	C3*	A	C1088	6.153	9.200	-3.261	1.00	27.75	RNA1	C
ATOM	2325	O3*	A	C1088	6.465	7.951	-3.847	1.00	19.39	RNA1	O
ATOM	2326	C2*	A	C1088	4.848	9.717	-3.842	1.00	20.69	RNA1	C
ATOM	2327	O2*	A	C1088	4.730	9.462	-5.224	1.00	39.54	RNA1	O
ATOM	2328	C1*	A	C1088	3.821	8.926	-3.035	1.00	19.38	RNA1	C
ATOM	2329	N9	A	C1088	2.553	9.623	-2.868	1.00	12.67	RNA1	N
ATOM	2330	C8	A	C1088	1.291	9.132	-3.089	1.00	19.49	RNA1	C
ATOM	2331	N7	A	C1088	0.338	9.996	-2.842	1.00	19.80	RNA1	N
ATOM	2332	C5	A	C1088	1.019	11.134	-2.432	1.00	11.03	RNA1	C

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ATOM  2333  C6   A C1088     0.578  12.406  -2.033  1.00 14.84      RNA1 C
ATOM  2334  N6   A C1088    -0.708  12.768  -1.988  1.00 13.38      RNA1 N
ATOM  2335  N1   A C1088     1.517  13.309  -1.680  1.00 16.35      RNA1 N
ATOM  2336  C2   A C1088     2.807  12.952  -1.736  1.00 16.68      RNA1 C
ATOM  2337  N3   A C1088     3.343  11.792  -2.099  1.00 19.47      RNA1 N
ATOM  2338  C4   A C1088     2.383  10.917  -2.440  1.00 11.60      RNA1 C
ATOM  2339  P    G C1089     7.282   7.896  -5.216  1.00 26.48      RNA1 P
ATOM  2340  O1P  G C1089     7.768   9.270  -5.525  1.00 30.79      RNA1 O
ATOM  2341  O2P  G C1089     6.437   7.171  -6.198  1.00 18.45      RNA1 O
ATOM  2342  O5*  G C1089     8.548   7.011  -4.853  1.00 14.93      RNA1 O
ATOM  2343  C5*  G C1089     9.568   7.515  -3.971  1.00 29.50      RNA1 C
ATOM  2344  C4*  G C1089    10.362   6.367  -3.400  1.00 26.25      RNA1 C
ATOM  2345  O4*  G C1089     9.469   5.554  -2.600  1.00 34.26      RNA1 O
ATOM  2346  C3*  G C1089    10.981   5.439  -4.439  1.00 20.63      RNA1 C
ATOM  2347  O3*  G C1089    12.197   4.922  -3.925  1.00 28.79      RNA1 O
ATOM  2348  C2*  G C1089     9.965   4.305  -4.531  1.00 28.82      RNA1 C
ATOM  2349  O2*  G C1089    10.543   3.072  -4.908  1.00 40.76      RNA1 O
ATOM  2350  C1*  G C1089     9.439   4.238  -3.099  1.00 19.76      RNA1 C
ATOM  2351  N9   G C1089     8.069   3.749  -2.988  1.00 15.09      RNA1 N
ATOM  2352  C8   G C1089     6.930   4.499  -2.817  1.00 17.24      RNA1 C
ATOM  2353  N7   G C1089     5.848   3.773  -2.729  1.00 20.25      RNA1 N
ATOM  2354  C5   G C1089     6.301   2.466  -2.857  1.00 14.36      RNA1 C
ATOM  2355  C6   G C1089     5.590   1.243  -2.839  1.00 23.53      RNA1 C
ATOM  2356  O6   G C1089     4.368   1.060  -2.704  1.00 38.04      RNA1 O
ATOM  2357  N1   G C1089     6.442   0.156  -2.998  1.00 10.56      RNA1 N
ATOM  2358  C2   G C1089     7.801   0.235  -3.159  1.00 16.75      RNA1 C
ATOM  2359  N2   G C1089     8.456  -0.931  -3.305  1.00 18.05      RNA1 N
ATOM  2360  N3   G C1089     8.475   1.369  -3.178  1.00 14.70      RNA1 N
ATOM  2361  C4   G C1089     7.668   2.437  -3.022  1.00 10.92      RNA1 C
ATOM  2362  P    U C1090    13.585   5.675  -4.221  1.00 43.14      RNA1 P
ATOM  2363  O1P  U C1090    13.436   6.453  -5.476  1.00 42.35      RNA1 O
ATOM  2364  O2P  U C1090    14.010   6.371  -2.971  1.00 42.92      RNA1 O
ATOM  2365  O5*  U C1090    14.587   4.467  -4.490  1.00 39.62      RNA1 O
ATOM  2366  C5*  U C1090    15.989   4.585  -4.207  1.00 45.78      RNA1 C
ATOM  2367  C4*  U C1090    16.693   3.275  -4.492  1.00 55.27      RNA1 C
ATOM  2368  O4*  U C1090    16.237   2.246  -3.570  1.00 55.21      RNA1 O
ATOM  2369  C3*  U C1090    16.455   2.661  -5.862  1.00 53.66      RNA1 C
ATOM  2370  O3*  U C1090    17.267   3.222  -6.875  1.00 51.89      RNA1 O
ATOM  2371  C2*  U C1090    16.781   1.194  -5.637  1.00 48.18      RNA1 C
ATOM  2372  O2*  U C1090    18.172   0.949  -5.690  1.00 54.31      RNA1 O
ATOM  2373  C1*  U C1090    16.271   0.979  -4.213  1.00 41.15      RNA1 C
ATOM  2374  N1   U C1090    14.922   0.387  -4.190  1.00 41.07      RNA1 N
ATOM  2375  C2   U C1090    14.823  -0.998  -4.283  1.00 36.51      RNA1 C
ATOM  2376  O2   U C1090    15.792  -1.730  -4.388  1.00 37.99      RNA1 O
ATOM  2377  N3   U C1090    13.542  -1.493  -4.256  1.00 24.06      RNA1 N
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ATOM  2378  C4   U C1090    12.374  -0.772  -4.150  1.00 29.36      RNA1 C
ATOM  2379  O4   U C1090    11.297  -1.373  -4.078  1.00 32.44      RNA1 O
ATOM  2380  C5   U C1090    12.554   0.649  -4.068  1.00 27.73      RNA1 C
ATOM  2381  C6   U C1090    13.788   1.167  -4.087  1.00 33.24      RNA1 C
ATOM  2382  P    G C1091    16.725   3.245  -8.383  1.00 58.06      RNA1 P
ATOM  2383  O1P  G C1091    15.277   3.599  -8.351  1.00 49.18      RNA1 O
ATOM  2384  O2P  G C1091    17.668   4.074  -9.177  1.00 62.85      RNA1 O
ATOM  2385  O5*  G C1091    16.838   1.724  -8.851  1.00 59.36      RNA1 O
ATOM  2386  C5*  G C1091    18.123   1.141  -9.135  1.00 62.76      RNA1 C
ATOM  2387  C4*  G C1091    18.029  -0.370  -9.212  1.00 62.76      RNA1 C
ATOM  2388  O4*  G C1091    17.448  -0.882  -7.980  1.00 57.83      RNA1 O
ATOM  2389  C3*  G C1091    17.168  -0.998 -10.302  1.00 67.15      RNA1 C
ATOM  2390  O3*  G C1091    17.800  -1.073 -11.581  1.00 73.47      RNA1 O
ATOM  2391  C2*  G C1091    16.911  -2.391  -9.736  1.00 63.68      RNA1 C
ATOM  2392  O2*  G C1091    17.997  -3.276  -9.939  1.00 66.38      RNA1 O
ATOM  2393  C1*  G C1091    16.766  -2.098  -8.243  1.00 52.76      RNA1 C
ATOM  2394  N9   G C1091    15.354  -1.954  -7.902  1.00 42.68      RNA1 N
ATOM  2395  C8   G C1091    14.638  -0.795  -7.717  1.00 43.79      RNA1 C
ATOM  2396  N7   G C1091    13.368  -1.009  -7.490  1.00 42.36      RNA1 N
ATOM  2397  C5   G C1091    13.243  -2.392  -7.512  1.00 31.07      RNA1 C
ATOM  2398  C6   G C1091    12.100  -3.220  -7.342  1.00 32.80      RNA1 C
ATOM  2399  O6   G C1091    10.926  -2.886  -7.133  1.00 29.29      RNA1 O
ATOM  2400  N1   G C1091    12.427  -4.567  -7.442  1.00 27.53      RNA1 N
ATOM  2401  C2   G C1091    13.687  -5.057  -7.676  1.00 37.58      RNA1 C
ATOM  2402  N2   G C1091    13.806  -6.387  -7.734  1.00 43.37      RNA1 N
ATOM  2403  N3   G C1091    14.754  -4.300  -7.840  1.00 37.83      RNA1 N
ATOM  2404  C4   G C1091    14.461  -2.989  -7.748  1.00 34.74      RNA1 C
ATOM  2405  P    C C1092    16.901  -1.334 -12.902  1.00 78.16      RNA1 P
ATOM  2406  O1P  C C1092    15.717  -0.429 -12.869  1.00 76.90      RNA1 O
ATOM  2407  O2P  C C1092    17.813  -1.307 -14.079  1.00 77.44      RNA1 O
ATOM  2408  O5*  C C1092    16.360  -2.822 -12.721  1.00 69.64      RNA1 O
ATOM  2409  C5*  C C1092    17.277  -3.929 -12.693  1.00 63.11      RNA1 C
ATOM  2410  C4*  C C1092    16.536  -5.243 -12.604  1.00 59.28      RNA1 C
ATOM  2411  O4*  C C1092    15.859  -5.364 -11.322  1.00 50.31      RNA1 O
ATOM  2412  C3*  C C1092    15.433  -5.487 -13.621  1.00 60.54      RNA1 C
ATOM  2413  O3*  C C1092    15.910  -5.898 -14.893  1.00 61.03      RNA1 O
ATOM  2414  C2*  C C1092    14.614  -6.580 -12.949  1.00 56.00      RNA1 C
ATOM  2415  O2*  C C1092    15.155  -7.875 -13.128  1.00 59.60      RNA1 O
ATOM  2416  C1*  C C1092    14.704  -6.175 -11.477  1.00 46.68      RNA1 C
ATOM  2417  N1   C C1092    13.500  -5.411 -11.103  1.00 45.69      RNA1 N
ATOM  2418  C2   C C1092    12.311  -6.125 -10.845  1.00 48.75      RNA1 C
ATOM  2419  O2   C C1092    12.334  -7.367 -10.877  1.00 35.22      RNA1 O
ATOM  2420  N3   C C1092    11.175  -5.443 -10.568  1.00 40.06      RNA1 N
ATOM  2421  C4   C C1092    11.191  -4.109 -10.529  1.00 43.65      RNA1 C
ATOM  2422  N4   C C1092    10.043  -3.483 -10.269  1.00 38.14      RNA1 N
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ATOM	2423	C5	C	C1092	12.386	-3.357	-10.759	1.00	43.83	RNA1 C
ATOM	2424	C6	C	C1092	13.508	-4.043	-11.036	1.00	48.70	RNA1 C
ATOM	2425	P	G	C1093	15.082	-5.497	-16.210	1.00	59.69	RNA1 P
ATOM	2426	O1P	G	C1093	14.954	-4.014	-16.213	1.00	64.26	RNA1 O
ATOM	2427	O2P	G	C1093	15.706	-6.182	-17.376	1.00	68.36	RNA1 O
ATOM	2428	O5*	G	C1093	13.629	-6.109	-15.961	1.00	39.18	RNA1 O
ATOM	2429	C5*	G	C1093	13.440	-7.525	-15.810	1.00	34.94	RNA1 C
ATOM	2430	C4*	G	C1093	12.017	-7.828	-15.395	1.00	40.12	RNA1 C
ATOM	2431	O4*	G	C1093	11.737	-7.199	-14.117	1.00	45.67	RNA1 O
ATOM	2432	C3*	G	C1093	10.929	-7.304	-16.315	1.00	43.53	RNA1 C
ATOM	2433	O3*	G	C1093	10.687	-8.168	-17.410	1.00	48.03	RNA1 O
ATOM	2434	C2*	G	C1093	9.720	-7.183	-15.391	1.00	41.69	RNA1 C
ATOM	2435	O2*	G	C1093	8.996	-8.389	-15.229	1.00	27.92	RNA1 O
ATOM	2436	C1*	G	C1093	10.381	-6.769	-14.075	1.00	38.16	RNA1 C
ATOM	2437	N9	G	C1093	10.350	-5.318	-13.870	1.00	36.77	RNA1 N
ATOM	2438	C8	G	C1093	11.401	-4.431	-13.970	1.00	34.83	RNA1 C
ATOM	2439	N7	G	C1093	11.048	-3.190	-13.762	1.00	32.06	RNA1 N
ATOM	2440	C5	G	C1093	9.685	-3.259	-13.505	1.00	27.72	RNA1 C
ATOM	2441	C6	G	C1093	8.752	-2.231	-13.223	1.00	27.54	RNA1 C
ATOM	2442	O6	G	C1093	8.947	-1.013	-13.160	1.00	34.45	RNA1 O
ATOM	2443	N1	G	C1093	7.475	-2.743	-13.014	1.00	19.53	RNA1 N
ATOM	2444	C2	G	C1093	7.136	-4.075	-13.075	1.00	19.64	RNA1 C
ATOM	2445	N2	G	C1093	5.851	-4.382	-12.830	1.00	17.24	RNA1 N
ATOM	2446	N3	G	C1093	7.993	-5.040	-13.352	1.00	21.92	RNA1 N
ATOM	2447	C4	G	C1093	9.241	-4.566	-13.554	1.00	25.99	RNA1 C
ATOM	2448	P	U	C1094	10.214	-7.545	-18.808	1.00	48.86	RNA1 P
ATOM	2449	O1P	U	C1094	11.019	-6.314	-19.033	1.00	51.40	RNA1 O
ATOM	2450	O2P	U	C1094	10.225	-8.631	-19.820	1.00	62.99	RNA1 O
ATOM	2451	O5*	U	C1094	8.700	-7.137	-18.549	1.00	35.14	RNA1 O
ATOM	2452	C5*	U	C1094	7.726	-8.151	-18.319	1.00	39.65	RNA1 C
ATOM	2453	C4*	U	C1094	6.342	-7.561	-18.289	1.00	45.60	RNA1 C
ATOM	2454	O4*	U	C1094	6.086	-6.907	-17.022	1.00	47.84	RNA1 O
ATOM	2455	C3*	U	C1094	6.030	-6.503	-19.328	1.00	46.03	RNA1 C
ATOM	2456	O3*	U	C1094	5.775	-7.078	-20.601	1.00	56.79	RNA1 O
ATOM	2457	C2*	U	C1094	4.829	-5.786	-18.713	1.00	44.04	RNA1 C
ATOM	2458	O2*	U	C1094	3.588	-6.431	-18.943	1.00	37.76	RNA1 O
ATOM	2459	C1*	U	C1094	5.168	-5.844	-17.219	1.00	44.47	RNA1 C
ATOM	2460	N1	U	C1094	5.770	-4.589	-16.742	1.00	26.87	RNA1 N
ATOM	2461	C2	U	C1094	4.909	-3.585	-16.329	1.00	22.09	RNA1 C
ATOM	2462	O2	U	C1094	3.691	-3.719	-16.288	1.00	25.93	RNA1 O
ATOM	2463	N3	U	C1094	5.519	-2.419	-15.962	1.00	13.38	RNA1 N
ATOM	2464	C4	U	C1094	6.869	-2.159	-15.947	1.00	36.16	RNA1 C
ATOM	2465	O4	U	C1094	7.263	-1.036	-15.621	1.00	36.16	RNA1 O
ATOM	2466	C5	U	C1094	7.696	-3.256	-16.357	1.00	27.39	RNA1 C
ATOM	2467	C6	U	C1094	7.131	-4.404	-16.729	1.00	19.00	RNA1 C

ATOM	2468	P	A	C1095	6.404	-6.394	-21.913	1.00 56.22	RNA1 P
ATOM	2469	O1P	A	C1095	7.761	-5.866	-21.571	1.00 36.24	RNA1 O
ATOM	2470	O2P	A	C1095	6.257	-7.345	-23.045	1.00 62.45	RNA1 O
ATOM	2471	O5*	A	C1095	5.420	-5.169	-22.156	1.00 37.34	RNA1 O
ATOM	2472	C5*	A	C1095	5.858	-3.993	-22.836	1.00 26.88	RNA1 C
ATOM	2473	C4*	A	C1095	4.732	-3.002	-22.897	1.00 25.01	RNA1 C
ATOM	2474	O4*	A	C1095	3.576	-3.668	-23.451	1.00 31.13	RNA1 O
ATOM	2475	C3*	A	C1095	4.254	-2.489	-21.555	1.00 30.12	RNA1 C
ATOM	2476	O3*	A	C1095	5.068	-1.403	-21.134	1.00 47.22	RNA1 O
ATOM	2477	C2*	A	C1095	2.797	-2.116	-21.824	1.00 32.85	RNA1 C
ATOM	2478	O2*	A	C1095	2.630	-0.839	-22.418	1.00 29.79	RNA1 O
ATOM	2479	C1*	A	C1095	2.395	-3.179	-22.845	1.00 21.93	RNA1 C
ATOM	2480	N9	A	C1095	1.649	-4.328	-22.333	1.00 17.01	RNA1 N
ATOM	2481	C8	A	C1095	2.142	-5.568	-21.985	1.00 21.36	RNA1 C
ATOM	2482	N7	A	C1095	1.211	-6.424	-21.627	1.00 21.32	RNA1 N
ATOM	2483	C5	A	C1095	0.031	-5.696	-21.729	1.00 10.86	RNA1 C
ATOM	2484	C6	A	C1095	-1.315	-6.037	-21.498	1.00 23.82	RNA1 C
ATOM	2485	N6	A	C1095	-1.717	-7.254	-21.118	1.00 35.80	RNA1 N
ATOM	2486	N1	A	C1095	-2.249	-5.076	-21.679	1.00 30.20	RNA1 N
ATOM	2487	C2	A	C1095	-1.844	-3.861	-22.076	1.00 23.15	RNA1 C
ATOM	2488	N3	A	C1095	-0.610	-3.423	-22.337	1.00 20.47	RNA1 N
ATOM	2489	C4	A	C1095	0.289	-4.399	-22.143	1.00 9.00	RNA1 C
ATOM	2490	P	A	C1096	5.554	-1.325	-19.607	1.00 33.71	RNA1 P
ATOM	2491	O1P	A	C1096	5.985	-2.689	-19.209	1.00 38.06	RNA1 O
ATOM	2492	O2P	A	C1096	6.505	-0.198	-19.472	1.00 30.42	RNA1 O
ATOM	2493	O5*	A	C1096	4.203	-0.950	-18.856	1.00 19.71	RNA1 O
ATOM	2494	C5*	A	C1096	3.610	0.332	-19.065	1.00 17.59	RNA1 C
ATOM	2495	C4*	A	C1096	2.176	0.335	-18.609	1.00 25.20	RNA1 C
ATOM	2496	O4*	A	C1096	1.399	-0.548	-19.452	1.00 36.18	RNA1 O
ATOM	2497	C3*	A	C1096	1.916	-0.155	-17.197	1.00 31.52	RNA1 C
ATOM	2498	O3*	A	C1096	2.158	0.858	-16.224	1.00 40.13	RNA1 O
ATOM	2499	C2*	A	C1096	0.458	-0.589	-17.277	1.00 29.94	RNA1 C
ATOM	2500	O2*	A	C1096	-0.436	0.497	-17.220	1.00 33.53	RNA1 O
ATOM	2501	C1*	A	C1096	0.392	-1.181	-18.684	1.00 28.76	RNA1 C
ATOM	2502	N9	A	C1096	0.682	-2.615	-18.662	1.00 29.57	RNA1 N
ATOM	2503	C8	A	C1096	1.915	-3.230	-18.760	1.00 20.07	RNA1 C
ATOM	2504	N7	A	C1096	1.862	-4.536	-18.673	1.00 16.60	RNA1 N
ATOM	2505	C5	A	C1096	0.506	-4.803	-18.515	1.00 21.73	RNA1 C
ATOM	2506	C6	A	C1096	-0.207	-6.004	-18.372	1.00 21.62	RNA1 C
ATOM	2507	N6	A	C1096	0.376	-7.207	-18.386	1.00 30.29	RNA1 N
ATOM	2508	N1	A	C1096	-1.551	-5.928	-18.222	1.00 19.53	RNA1 N
ATOM	2509	C2	A	C1096	-2.130	-4.715	-18.234	1.00 19.83	RNA1 C
ATOM	2510	N3	A	C1096	-1.565	-3.512	-18.377	1.00 21.31	RNA1 N
ATOM	2511	C4	A	C1096	-0.231	-3.630	-18.511	1.00 13.07	RNA1 C
ATOM	2512	P	C	C1097	2.770	0.451	-14.795	1.00 34.58	RNA1 P

ATOM 2513 O1P C C1097 3.901 -0.488 -15.013 1.00 24.95 RNA1 O
ATOM 2514 O2P C C1097 3.010 1.716 -14.062 1.00 42.37 RNA1 O
ATOM 2515 O5* C C1097 1.558 -0.333 -14.115 1.00 33.44 RNA1 O
ATOM 2516 C5* C C1097 1.711 -1.664 -13.564 1.00 27.30 RNA1 C
ATOM 2517 C4* C C1097 0.347 -2.298 -13.386 1.00 34.16 RNA1 C
ATOM 2518 O4* C C1097 -0.067 -2.943 -14.625 1.00 37.39 RNA1 O
ATOM 2519 C3* C C1097 0.219 -3.406 -12.354 1.00 33.88 RNA1 C
ATOM 2520 O3* C C1097 0.093 -2.924 -11.025 1.00 36.37 RNA1 O
ATOM 2521 C2* C C1097 -1.041 -4.120 -12.816 1.00 36.19 RNA1 C
ATOM 2522 O2* C C1097 -2.214 -3.415 -12.457 1.00 31.86 RNA1 O
ATOM 2523 C1* C C1097 -0.865 -4.089 -14.334 1.00 35.36 RNA1 C
ATOM 2524 N1 C C1097 -0.146 -5.311 -14.780 1.00 29.78 RNA1 N
ATOM 2525 C2 C C1097 -0.859 -6.537 -14.895 1.00 31.29 RNA1 C
ATOM 2526 O2 C C1097 -2.097 -6.552 -14.732 1.00 30.74 RNA1 O
ATOM 2527 N3 C C1097 -0.175 -7.667 -15.188 1.00 27.52 RNA1 N
ATOM 2528 C4 C C1097 1.146 -7.616 -15.390 1.00 35.55 RNA1 C
ATOM 2529 N4 C C1097 1.788 -8.764 -15.640 1.00 38.53 RNA1 N
ATOM 2530 C5 C C1097 1.874 -6.389 -15.338 1.00 27.77 RNA1 C
ATOM 2531 C6 C C1097 1.197 -5.275 -15.036 1.00 24.47 RNA1 C
ATOM 2532 P A C1098 1.072 -3.493 -9.886 1.00 38.47 RNA1 P
ATOM 2533 O1P A C1098 2.477 -3.131 -10.212 1.00 22.01 RNA1 O
ATOM 2534 O2P A C1098 0.484 -3.068 -8.588 1.00 56.40 RNA1 O
ATOM 2535 O5* A C1098 0.959 -5.079 -10.023 1.00 40.54 RNA1 O
ATOM 2536 C5* A C1098 -0.328 -5.740 -9.972 1.00 47.03 RNA1 C
ATOM 2537 C4* A C1098 -0.192 -7.201 -10.348 1.00 50.05 RNA1 C
ATOM 2538 O4* A C1098 0.276 -7.310 -11.720 1.00 43.04 RNA1 O
ATOM 2539 C3* A C1098 0.819 -8.007 -9.544 1.00 59.35 RNA1 C
ATOM 2540 O3* A C1098 0.289 -8.467 -8.305 1.00 57.94 RNA1 O
ATOM 2541 C2* A C1098 1.170 -9.146 -10.496 1.00 54.42 RNA1 C
ATOM 2542 O2* A C1098 0.229 -10.203 -10.479 1.00 63.88 RNA1 O
ATOM 2543 C1* A C1098 1.125 -8.440 -11.851 1.00 42.41 RNA1 C
ATOM 2544 N9 A C1098 2.456 -7.982 -12.247 1.00 29.98 RNA1 N
ATOM 2545 C8 A C1098 2.967 -6.709 -12.213 1.00 32.72 RNA1 C
ATOM 2546 N7 A C1098 4.222 -6.633 -12.588 1.00 34.32 RNA1 N
ATOM 2547 C5 A C1098 4.557 -7.942 -12.902 1.00 34.44 RNA1 C
ATOM 2548 C6 A C1098 5.751 -8.533 -13.363 1.00 43.55 RNA1 C
ATOM 2549 N6 A C1098 6.879 -7.852 -13.597 1.00 39.58 RNA1 N
ATOM 2550 N1 A C1098 5.746 -9.866 -13.579 1.00 48.91 RNA1 N
ATOM 2551 C2 A C1098 4.615 -10.549 -13.348 1.00 42.95 RNA1 C
ATOM 2552 N3 A C1098 3.435 -10.108 -12.916 1.00 35.82 RNA1 N
ATOM 2553 C4 A C1098 3.474 -8.782 -12.708 1.00 35.65 RNA1 C
ATOM 2554 P G C1099 1.238 -8.516 -7.006 1.00 52.26 RNA1 P
ATOM 2555 O1P G C1099 1.696 -7.137 -6.706 1.00 52.99 RNA1 O
ATOM 2556 O2P G C1099 0.511 -9.287 -5.970 1.00 54.62 RNA1 O
ATOM 2557 O5* G C1099 2.513 -9.346 -7.481 1.00 43.47 RNA1 O

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ATOM  2558 C5*  G C1099     2.413 -10.749  -7.772  1.00 41.68      RNA1 C
ATOM  2559 C4*  G C1099     3.735 -11.273  -8.271  1.00 42.05      RNA1 C
ATOM  2560 O4*  G C1099     4.033 -10.671  -9.554  1.00 43.83      RNA1 O
ATOM  2561 C3*  G C1099     4.938 -10.934  -7.409  1.00 48.09      RNA1 C
ATOM  2562 O3*  G C1099     5.100 -11.821  -6.317  1.00 58.27      RNA1 O
ATOM  2563 C2*  G C1099     6.089 -10.992  -8.402  1.00 50.43      RNA1 C
ATOM  2564 O2*  G C1099     6.588 -12.296  -8.639  1.00 57.02      RNA1 O
ATOM  2565 C1*  G C1099     5.426 -10.432  -9.660  1.00 44.89      RNA1 C
ATOM  2566 N9   G C1099     5.639  -8.989  -9.729  1.00 45.65      RNA1 N
ATOM  2567 C8   G C1099     4.714  -7.993  -9.515  1.00 38.56      RNA1 C
ATOM  2568 N7   G C1099     5.228  -6.796  -9.584  1.00 41.94      RNA1 N
ATOM  2569 C5   G C1099     6.569  -7.014  -9.873  1.00 34.92      RNA1 C
ATOM  2570 C6   G C1099     7.631  -6.094 -10.053  1.00 42.48      RNA1 C
ATOM  2571 O6   G C1099     7.601  -4.857  -9.985  1.00 44.46      RNA1 O
ATOM  2572 N1   G C1099     8.829  -6.746 -10.336  1.00 41.82      RNA1 N
ATOM  2573 C2   G C1099     8.982  -8.108 -10.437  1.00 42.77      RNA1 C
ATOM  2574 N2   G C1099    10.211  -8.548 -10.736  1.00 31.50      RNA1 N
ATOM  2575 N3   G C1099     8.001  -8.974 -10.262  1.00 31.12      RNA1 N
ATOM  2576 C4   G C1099     6.832  -8.362  -9.984  1.00 33.36      RNA1 C
ATOM  2577 P    C C1100     5.772 -11.286  -4.956  1.00 62.31      RNA1 P
ATOM  2578 O1P  C C1100     5.270  -9.914  -4.687  1.00 56.23      RNA1 O
ATOM  2579 O2P  C C1100     5.583 -12.348  -3.934  1.00 65.10      RNA1 O
ATOM  2580 O5*  C C1100     7.320 -11.188  -5.316  1.00 45.54      RNA1 O
ATOM  2581 C5*  C C1100     8.052 -12.366  -5.670  1.00 43.72      RNA1 C
ATOM  2582 C4*  C C1100     9.458 -12.015  -6.069  1.00 40.97      RNA1 C
ATOM  2583 O4*  C C1100     9.429 -11.213  -7.276  1.00 44.70      RNA1 O
ATOM  2584 C3*  C C1100    10.249 -11.173  -5.087  1.00 43.30      RNA1 C
ATOM  2585 O3*  C C1100    10.817 -11.913  -4.022  1.00 57.32      RNA1 O
ATOM  2586 C2*  C C1100    11.306 -10.543  -5.980  1.00 45.40      RNA1 C
ATOM  2587 O2*  C C1100    12.407 -11.390  -6.236  1.00 41.08      RNA1 O
ATOM  2588 C1*  C C1100    10.508 -10.293  -7.258  1.00 40.42      RNA1 C
ATOM  2589 N1   C C1100     9.968  -8.923  -7.239  1.00 34.22      RNA1 N
ATOM  2590 C2   C C1100    10.851  -7.860  -7.450  1.00 34.09      RNA1 C
ATOM  2591 O2   C C1100    12.043  -8.112  -7.698  1.00 30.44      RNA1 O
ATOM  2592 N3   C C1100    10.390  -6.595  -7.377  1.00 32.20      RNA1 N
ATOM  2593 C4   C C1100     9.102  -6.369  -7.112  1.00 36.06      RNA1 C
ATOM  2594 N4   C C1100     8.695  -5.101  -7.023  1.00 42.37      RNA1 N
ATOM  2595 C5   C C1100     8.173  -7.432  -6.920  1.00 31.00      RNA1 C
ATOM  2596 C6   C C1100     8.643  -8.681  -6.995  1.00 29.98      RNA1 C
ATOM  2597 P    U C1101    11.026 -11.199  -2.592  1.00 60.70      RNA1 P
ATOM  2598 O1P  U C1101     9.727 -10.588  -2.196  1.00 50.26      RNA1 O
ATOM  2599 O2P  U C1101    11.694 -12.160  -1.673  1.00 70.90      RNA1 O
ATOM  2600 O5*  U C1101    12.055 -10.024  -2.904  1.00 44.87      RNA1 O
ATOM  2601 C5*  U C1101    13.364 -10.316  -3.411  1.00 39.54      RNA1 C
ATOM  2602 C4*  U C1101    14.139  -9.041  -3.619  1.00 45.93      RNA1 C
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ATOM  2603  O4*  U C1101     13.487  -8.234  -4.635  1.00 53.56      RNA1 O
ATOM  2604  C3*  U C1101     14.232  -8.111  -2.424  1.00 45.04      RNA1 C
ATOM  2605  O3*  U C1101     15.241  -8.491  -1.503  1.00 55.35      RNA1 O
ATOM  2606  C2*  U C1101     14.519  -6.767  -3.078  1.00 45.97      RNA1 C
ATOM  2607  O2*  U C1101     15.875  -6.620  -3.450  1.00 43.86      RNA1 O
ATOM  2608  C1*  U C1101     13.668  -6.856  -4.341  1.00 43.43      RNA1 C
ATOM  2609  N1   U C1101     12.349  -6.220  -4.172  1.00 40.87      RNA1 N
ATOM  2610  C2   U C1101     12.289  -4.831  -4.234  1.00 35.67      RNA1 C
ATOM  2611  O2   U C1101     13.277  -4.130  -4.420  1.00 34.43      RNA1 O
ATOM  2612  N3   U C1101     11.032  -4.294  -4.067  1.00 27.89      RNA1 N
ATOM  2613  C4   U C1101      9.851  -4.983  -3.852  1.00 38.34      RNA1 C
ATOM  2614  O4   U C1101      8.792  -4.355  -3.727  1.00 30.79      RNA1 O
ATOM  2615  C5   U C1101      9.993  -6.408  -3.801  1.00 38.67      RNA1 C
ATOM  2616  C6   U C1101     11.204  -6.965  -3.959  1.00 40.99      RNA1 C
ATOM  2617  P    C C1102     15.110  -8.040   0.038  1.00 56.93      RNA1 P
ATOM  2618  O1P  C C1102     13.690  -8.220   0.458  1.00 45.32      RNA1 O
ATOM  2619  O2P  C C1102     16.195  -8.697   0.810  1.00 59.07      RNA1 O
ATOM  2620  O5*  C C1102     15.415  -6.479   0.002  1.00 47.10      RNA1 O
ATOM  2621  C5*  C C1102     16.687  -6.002  -0.447  1.00 40.92      RNA1 C
ATOM  2622  C4*  C C1102     16.706  -4.495  -0.480  1.00 41.54      RNA1 C
ATOM  2623  O4*  C C1102     15.809  -4.001  -1.511  1.00 45.86      RNA1 O
ATOM  2624  C3*  C C1102     16.235  -3.772   0.769  1.00 43.22      RNA1 C
ATOM  2625  O3*  C C1102     17.189  -3.732   1.814  1.00 49.70      RNA1 O
ATOM  2626  C2*  C C1102     15.910  -2.389   0.227  1.00 45.44      RNA1 C
ATOM  2627  O2*  C C1102     17.061  -1.587   0.031  1.00 39.52      RNA1 O
ATOM  2628  C1*  C C1102     15.294  -2.733  -1.125  1.00 41.32      RNA1 C
ATOM  2629  N1   C C1102     13.822  -2.807  -1.006  1.00 35.07      RNA1 N
ATOM  2630  C2   C C1102     13.091  -1.607  -0.999  1.00 35.73      RNA1 C
ATOM  2631  O2   C C1102     13.700  -0.530  -1.134  1.00 40.70      RNA1 O
ATOM  2632  N3   C C1102     11.748  -1.649  -0.843  1.00 24.21      RNA1 N
ATOM  2633  C4   C C1102     11.131  -2.821  -0.703  1.00 25.56      RNA1 C
ATOM  2634  N4   C C1102      9.805  -2.813  -0.534  1.00 27.04      RNA1 N
ATOM  2635  C5   C C1102     11.844  -4.056  -0.726  1.00 25.22      RNA1 C
ATOM  2636  C6   C C1102     13.175  -4.004  -0.880  1.00 29.24      RNA1 C
ATOM  2637  P    A C1103     16.678  -3.598   3.336  1.00 46.37      RNA1 P
ATOM  2638  O1P  A C1103     15.453  -4.431   3.507  1.00 34.79      RNA1 O
ATOM  2639  O2P  A C1103     17.841  -3.806   4.238  1.00 53.23      RNA1 O
ATOM  2640  O5*  A C1103     16.223  -2.077   3.443  1.00 50.88      RNA1 O
ATOM  2641  C5*  A C1103     17.095  -1.012   3.017  1.00 45.92      RNA1 C
ATOM  2642  C4*  A C1103     16.368   0.307   3.082  1.00 42.03      RNA1 C
ATOM  2643  O4*  A C1103     15.249   0.282   2.164  1.00 42.45      RNA1 O
ATOM  2644  C3*  A C1103     15.748   0.629   4.431  1.00 46.34      RNA1 C
ATOM  2645  O3*  A C1103     16.697   1.231   5.297  1.00 50.61      RNA1 O
ATOM  2646  C2*  A C1103     14.604   1.568   4.068  1.00 40.60      RNA1 C
ATOM  2647  O2*  A C1103     15.018   2.911   3.913  1.00 43.99      RNA1 O
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ATOM	2648	C1*	A C1103	14.163	1.007	2.714	1.00	35.23	RNA1	C
ATOM	2649	N9	A C1103	13.007	0.114	2.815	1.00	24.56	RNA1	N
ATOM	2650	C8	A C1103	12.964	-1.259	2.771	1.00	12.09	RNA1	C
ATOM	2651	N7	A C1103	11.755	-1.754	2.912	1.00	21.27	RNA1	N
ATOM	2652	C5	A C1103	10.949	-0.629	3.052	1.00	11.33	RNA1	C
ATOM	2653	C6	A C1103	9.566	-0.469	3.247	1.00	17.54	RNA1	C
ATOM	2654	N6	A C1103	8.699	-1.485	3.341	1.00	18.44	RNA1	N
ATOM	2655	N1	A C1103	9.091	0.792	3.351	1.00	23.77	RNA1	N
ATOM	2656	C2	A C1103	9.947	1.810	3.270	1.00	20.47	RNA1	C
ATOM	2657	N3	A C1103	11.262	1.789	3.093	1.00	25.40	RNA1	N
ATOM	2658	C4	A C1103	11.706	0.525	2.990	1.00	22.14	RNA1	C
ATOM	2659	P	C C1104	16.907	0.637	6.771	1.00	47.34	RNA1	P
ATOM	2660	O1P	C C1104	17.274	-0.801	6.656	1.00	47.39	RNA1	O
ATOM	2661	O2P	C C1104	17.809	1.572	7.493	1.00	49.59	RNA1	O
ATOM	2662	O5*	C C1104	15.454	0.717	7.410	1.00	32.80	RNA1	O
ATOM	2663	C5*	C C1104	14.847	1.985	7.660	1.00	32.89	RNA1	C
ATOM	2664	C4*	C C1104	13.409	1.804	8.055	1.00	33.67	RNA1	C
ATOM	2665	O4*	C C1104	12.654	1.301	6.924	1.00	36.61	RNA1	O
ATOM	2666	C3*	C C1104	13.151	0.793	9.157	1.00	44.60	RNA1	C
ATOM	2667	O3*	C C1104	13.379	1.321	10.455	1.00	47.83	RNA1	O
ATOM	2668	C2*	C C1104	11.699	0.409	8.912	1.00	41.50	RNA1	C
ATOM	2669	O2*	C C1104	10.802	1.363	9.443	1.00	39.51	RNA1	O
ATOM	2670	C1*	C C1104	11.635	0.426	7.382	1.00	35.38	RNA1	C
ATOM	2671	N1	C C1104	11.881	-0.915	6.818	1.00	26.79	RNA1	N
ATOM	2672	C2	C C1104	10.807	-1.804	6.699	1.00	30.49	RNA1	C
ATOM	2673	O2	C C1104	9.672	-1.426	7.039	1.00	25.17	RNA1	O
ATOM	2674	N3	C C1104	11.031	-3.049	6.216	1.00	35.06	RNA1	N
ATOM	2675	C4	C C1104	12.264	-3.412	5.850	1.00	35.48	RNA1	C
ATOM	2676	N4	C C1104	12.440	-4.649	5.381	1.00	39.73	RNA1	N
ATOM	2677	C5	C C1104	13.370	-2.524	5.948	1.00	26.28	RNA1	C
ATOM	2678	C6	C C1104	13.137	-1.298	6.432	1.00	26.38	RNA1	C
ATOM	2679	P	C C1105	13.943	0.357	11.610	1.00	45.15	RNA1	P
ATOM	2680	O1P	C C1105	14.937	-0.579	11.008	1.00	37.59	RNA1	O
ATOM	2681	O2P	C C1105	14.345	1.217	12.749	1.00	50.66	RNA1	O
ATOM	2682	O5*	C C1105	12.669	-0.496	12.036	1.00	27.84	RNA1	O
ATOM	2683	C5*	C C1105	11.541	0.141	12.636	1.00	26.44	RNA1	C
ATOM	2684	C4*	C C1105	10.431	-0.855	12.852	1.00	36.80	RNA1	C
ATOM	2685	O4*	C C1105	9.967	-1.354	11.569	1.00	46.02	RNA1	O
ATOM	2686	C3*	C C1105	10.793	-2.111	13.623	1.00	39.57	RNA1	C
ATOM	2687	O3*	C C1105	10.794	-1.905	15.026	1.00	48.60	RNA1	O
ATOM	2688	C2*	C C1105	9.713	-3.084	13.169	1.00	42.79	RNA1	C
ATOM	2689	O2*	C C1105	8.473	-2.848	13.811	1.00	36.52	RNA1	O
ATOM	2690	C1*	C C1105	9.576	-2.714	11.693	1.00	39.01	RNA1	C
ATOM	2691	N1	C C1105	10.448	-3.539	10.827	1.00	31.92	RNA1	N
ATOM	2692	C2	C C1105	10.029	-4.832	10.461	1.00	29.04	RNA1	C

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ATOM  2693  O2   C C1105     8.934  -5.259  10.875  1.00 27.41      RNA1 O
ATOM  2694  N3   C C1105    10.831  -5.584   9.672  1.00 26.50      RNA1 N
ATOM  2695  C4   C C1105    12.005  -5.100   9.255  1.00 26.95      RNA1 C
ATOM  2696  N4   C C1105    12.768  -5.879   8.473  1.00 32.01      RNA1 N
ATOM  2697  C5   C C1105    12.453  -3.798   9.614  1.00 31.44      RNA1 C
ATOM  2698  C6   C C1105    11.652  -3.059  10.389  1.00 27.18      RNA1 C
ATOM  2699  P    A C1106    11.685  -2.860  15.964  1.00 49.11      RNA1 P
ATOM  2700  O1P  A C1106    12.987  -3.106  15.282  1.00 36.36      RNA1 O
ATOM  2701  O2P  A C1106    11.676  -2.277  17.331  1.00 55.01      RNA1 O
ATOM  2702  O5*  A C1106    10.861  -4.222  15.988  1.00 33.45      RNA1 O
ATOM  2703  C5*  A C1106     9.507  -4.255  16.482  1.00 40.30      RNA1 C
ATOM  2704  C4*  A C1106     8.910  -5.628  16.280  1.00 55.66      RNA1 C
ATOM  2705  O4*  A C1106     8.774  -5.892  14.859  1.00 57.89      RNA1 O
ATOM  2706  C3*  A C1106     9.747  -6.785  16.804  1.00 61.21      RNA1 C
ATOM  2707  O3*  A C1106     9.552  -7.004  18.196  1.00 63.93      RNA1 O
ATOM  2708  C2*  A C1106     9.287  -7.945  15.928  1.00 60.31      RNA1 C
ATOM  2709  O2*  A C1106     8.040  -8.478  16.344  1.00 54.72      RNA1 O
ATOM  2710  C1*  A C1106     9.104  -7.244  14.582  1.00 50.43      RNA1 C
ATOM  2711  N9   A C1106    10.327  -7.245  13.772  1.00 40.12      RNA1 N
ATOM  2712  C8   A C1106    11.297  -6.265  13.730  1.00 43.18      RNA1 C
ATOM  2713  N7   A C1106    12.279  -6.522  12.899  1.00 35.92      RNA1 N
ATOM  2714  C5   A C1106    11.940  -7.754  12.356  1.00 35.80      RNA1 C
ATOM  2715  C6   A C1106    12.574  -8.570  11.401  1.00 32.97      RNA1 C
ATOM  2716  N6   A C1106    13.721  -8.242  10.791  1.00 42.58      RNA1 N
ATOM  2717  N1   A C1106    11.984  -9.744  11.088  1.00 28.98      RNA1 N
ATOM  2718  C2   A C1106    10.831 -10.065  11.694  1.00 37.34      RNA1 C
ATOM  2719  N3   A C1106    10.132  -9.379  12.601  1.00 37.05      RNA1 N
ATOM  2720  C4   A C1106    10.746  -8.218  12.893  1.00 37.35      RNA1 C
ATOM  2721  P    G C1107    10.770  -7.554  19.093  1.00 58.93      RNA1 P
ATOM  2722  O1P  G C1107    12.057  -7.023  18.562  1.00 36.85      RNA1 O
ATOM  2723  O2P  G C1107    10.406  -7.307  20.512  1.00 61.45      RNA1 O
ATOM  2724  O5*  G C1107    10.741  -9.124  18.823  1.00 57.72      RNA1 O
ATOM  2725  C5*  G C1107     9.559  -9.898  19.117  1.00 58.74      RNA1 C
ATOM  2726  C4*  G C1107     9.678 -11.278  18.520  1.00 65.40      RNA1 C
ATOM  2727  O4*  G C1107     9.633 -11.183  17.073  1.00 61.43      RNA1 O
ATOM  2728  C3*  G C1107    10.983 -11.999  18.818  1.00 66.79      RNA1 C
ATOM  2729  O3*  G C1107    10.969 -12.653  20.079  1.00 66.96      RNA1 O
ATOM  2730  C2*  G C1107    11.110 -12.966  17.647  1.00 65.40      RNA1 C
ATOM  2731  O2*  G C1107    10.392 -14.174  17.833  1.00 59.25      RNA1 O
ATOM  2732  C1*  G C1107    10.509 -12.142  16.504  1.00 56.87      RNA1 C
ATOM  2733  N9   G C1107    11.541 -11.428  15.759  1.00 46.90      RNA1 N
ATOM  2734  C8   G C1107    11.980 -10.140  15.964  1.00 49.14      RNA1 C
ATOM  2735  N7   G C1107    12.952  -9.797  15.163  1.00 45.19      RNA1 N
ATOM  2736  C5   G C1107    13.159 -10.921  14.374  1.00 43.33      RNA1 C
ATOM  2737  C6   G C1107    14.092 -11.155  13.326  1.00 44.94      RNA1 C
```

ATOM	2738	O6	G	C1107	14.953	-10.387	12.869	1.00	41.91	RNA1	O
ATOM	2739	N1	G	C1107	13.958	-12.437	12.803	1.00	44.05	RNA1	N
ATOM	2740	C2	G	C1107	13.048	-13.374	13.227	1.00	48.45	RNA1	C
ATOM	2741	N2	G	C1107	13.071	-14.553	12.597	1.00	49.02	RNA1	N
ATOM	2742	N3	G	C1107	12.177	-13.169	14.198	1.00	48.55	RNA1	N
ATOM	2743	C4	G	C1107	12.289	-11.932	14.725	1.00	47.37	RNA1	C
ATOM	2744	P	C	C1108	12.345	-12.840	20.886	1.00	71.15	RNA1	P
ATOM	2745	O1P	C	C1108	13.100	-11.558	20.849	1.00	59.46	RNA1	O
ATOM	2746	O2P	C	C1108	12.015	-13.463	22.194	1.00	75.00	RNA1	O
ATOM	2747	O5*	C	C1108	13.155	-13.893	20.010	1.00	72.84	RNA1	O
ATOM	2748	C5*	C	C1108	12.697	-15.251	19.876	1.00	75.04	RNA1	C
ATOM	2749	C4*	C	C1108	13.581	-16.004	18.914	1.00	76.03	RNA1	C
ATOM	2750	O4*	C	C1108	13.459	-15.420	17.592	1.00	73.82	RNA1	O
ATOM	2751	C3*	C	C1108	15.073	-15.954	19.208	1.00	77.22	RNA1	C
ATOM	2752	O3*	C	C1108	15.576	-16.622	20.377	1.00	76.14	RNA1	O
ATOM	2753	C2*	C	C1108	15.696	-16.220	17.844	1.00	77.82	RNA1	C
ATOM	2754	O2*	C	C1108	15.731	-17.593	17.507	1.00	80.53	RNA1	O
ATOM	2755	C1*	C	C1108	14.705	-15.511	16.916	1.00	74.18	RNA1	C
ATOM	2756	N1	C	C1108	15.147	-14.151	16.545	1.00	69.37	RNA1	N
ATOM	2757	C2	C	C1108	15.946	-13.987	15.400	1.00	64.11	RNA1	C
ATOM	2758	O2	C	C1108	16.232	-14.979	14.713	1.00	63.69	RNA1	O
ATOM	2759	N3	C	C1108	16.383	-12.750	15.074	1.00	59.38	RNA1	N
ATOM	2760	C4	C	C1108	16.047	-11.702	15.829	1.00	57.06	RNA1	C
ATOM	2761	N4	C	C1108	16.508	-10.503	15.472	1.00	58.03	RNA1	N
ATOM	2762	C5	C	C1108	15.224	-11.837	16.984	1.00	61.31	RNA1	C
ATOM	2763	C6	C	C1108	14.801	-13.066	17.303	1.00	67.15	RNA1	C
TER	2764		C	C1108							
ATOM	2765	O5*	G	D1051	13.368	11.108	-58.535	1.00	55.60	RNA2	O
ATOM	2766	C5*	G	D1051	14.100	12.302	-58.210	1.00	63.32	RNA2	C
ATOM	2767	C4*	G	D1051	13.550	13.505	-58.939	1.00	61.69	RNA2	C
ATOM	2768	O4*	G	D1051	13.809	13.364	-60.359	1.00	66.02	RNA2	O
ATOM	2769	C3*	G	D1051	12.043	13.659	-58.835	1.00	59.67	RNA2	C
ATOM	2770	O3*	G	D1051	11.661	14.349	-57.659	1.00	53.26	RNA2	O
ATOM	2771	C2*	G	D1051	11.684	14.404	-60.113	1.00	58.82	RNA2	C
ATOM	2772	O2*	G	D1051	11.873	15.801	-60.015	1.00	62.26	RNA2	O
ATOM	2773	C1*	G	D1051	12.691	13.815	-61.102	1.00	58.27	RNA2	C
ATOM	2774	N9	G	D1051	12.147	12.672	-61.833	1.00	55.11	RNA2	N
ATOM	2775	C8	G	D1051	12.505	11.352	-61.693	1.00	57.64	RNA2	C
ATOM	2776	N7	G	D1051	11.830	10.552	-62.472	1.00	63.74	RNA2	N
ATOM	2777	C5	G	D1051	10.976	11.393	-63.171	1.00	59.62	RNA2	C
ATOM	2778	C6	G	D1051	10.002	11.100	-64.162	1.00	54.61	RNA2	C
ATOM	2779	O6	G	D1051	9.687	9.999	-64.634	1.00	56.94	RNA2	O
ATOM	2780	N1	G	D1051	9.366	12.254	-64.606	1.00	52.85	RNA2	N
ATOM	2781	C2	G	D1051	9.629	13.525	-64.157	1.00	48.26	RNA2	C
ATOM	2782	N2	G	D1051	8.910	14.509	-64.707	1.00	49.20	RNA2	N

ATOM 2783 N3 G D1051 10.531 13.811 -63.237 1.00 51.58 RNA2 N
ATOM 2784 C4 G D1051 11.163 12.707 -62.791 1.00 56.30 RNA2 C
ATOM 2785 P C D1052 10.243 14.024 -56.983 1.00 59.48 RNA2 P
ATOM 2786 O1P C D1052 10.050 12.549 -57.013 1.00 61.66 RNA2 O
ATOM 2787 O2P C D1052 10.183 14.741 -55.688 1.00 73.92 RNA2 O
ATOM 2788 O5* C D1052 9.194 14.690 -57.976 1.00 41.41 RNA2 O
ATOM 2789 C5* C D1052 9.295 16.081 -58.307 1.00 47.28 RNA2 C
ATOM 2790 C4* C D1052 8.298 16.442 -59.376 1.00 45.31 RNA2 C
ATOM 2791 O4* C D1052 8.683 15.855 -60.645 1.00 50.63 RNA2 O
ATOM 2792 C3* C D1052 6.892 15.933 -59.137 1.00 47.61 RNA2 C
ATOM 2793 O3* C D1052 6.174 16.759 -58.247 1.00 56.07 RNA2 O
ATOM 2794 C2* C D1052 6.301 15.896 -60.540 1.00 49.42 RNA2 C
ATOM 2795 O2* C D1052 5.816 17.144 -60.990 1.00 40.34 RNA2 O
ATOM 2796 C1* C D1052 7.518 15.487 -61.371 1.00 50.98 RNA2 C
ATOM 2797 N1 C D1052 7.546 14.031 -61.621 1.00 53.95 RNA2 N
ATOM 2798 C2 C D1052 6.704 13.502 -62.611 1.00 53.59 RNA2 C
ATOM 2799 O2 C D1052 5.974 14.271 -63.253 1.00 52.10 RNA2 O
ATOM 2800 N3 C D1052 6.705 12.169 -62.838 1.00 59.04 RNA2 N
ATOM 2801 C4 C D1052 7.499 11.370 -62.120 1.00 65.70 RNA2 C
ATOM 2802 N4 C D1052 7.459 10.056 -62.374 1.00 66.17 RNA2 N
ATOM 2803 C5 C D1052 8.369 11.880 -61.110 1.00 59.37 RNA2 C
ATOM 2804 C6 C D1052 8.363 13.202 -60.898 1.00 55.97 RNA2 C
ATOM 2805 P U D1053 5.067 16.101 -57.298 1.00 63.43 RNA2 P
ATOM 2806 O1P U D1053 5.641 14.831 -56.780 1.00 62.31 RNA2 O
ATOM 2807 O2P U D1053 4.576 17.128 -56.343 1.00 74.13 RNA2 O
ATOM 2808 O5* U D1053 3.889 15.763 -58.312 1.00 57.11 RNA2 O
ATOM 2809 C5* U D1053 3.199 16.820 -58.990 1.00 48.12 RNA2 C
ATOM 2810 C4* U D1053 2.185 16.257 -59.953 1.00 50.31 RNA2 C
ATOM 2811 O4* U D1053 2.860 15.628 -61.074 1.00 49.75 RNA2 O
ATOM 2812 C3* U D1053 1.277 15.164 -59.421 1.00 50.89 RNA2 C
ATOM 2813 O3* U D1053 0.202 15.634 -58.629 1.00 56.33 RNA2 O
ATOM 2814 C2* U D1053 0.818 14.477 -60.698 1.00 50.72 RNA2 C
ATOM 2815 O2* U D1053 -0.225 15.175 -61.357 1.00 48.82 RNA2 O
ATOM 2816 C1* U D1053 2.091 14.528 -61.540 1.00 43.49 RNA2 C
ATOM 2817 N1 U D1053 2.881 13.292 -61.391 1.00 42.34 RNA2 N
ATOM 2818 C2 U D1053 2.501 12.182 -62.141 1.00 40.65 RNA2 C
ATOM 2819 O2 U D1053 1.564 12.193 -62.926 1.00 43.48 RNA2 O
ATOM 2820 N3 U D1053 3.258 11.057 -61.935 1.00 32.60 RNA2 N
ATOM 2821 C4 U D1053 4.329 10.920 -61.079 1.00 48.03 RNA2 C
ATOM 2822 O4 U D1053 4.880 9.822 -60.973 1.00 58.30 RNA2 O
ATOM 2823 C5 U D1053 4.670 12.106 -60.352 1.00 43.77 RNA2 C
ATOM 2824 C6 U D1053 3.954 13.222 -60.528 1.00 44.26 RNA2 C
ATOM 2825 P G D1054 -0.300 14.738 -57.393 1.00 63.07 RNA2 P
ATOM 2826 O1P G D1054 0.909 14.253 -56.659 1.00 56.57 RNA2 O
ATOM 2827 O2P G D1054 -1.342 15.504 -56.670 1.00 55.48 RNA2 O

ATOM	2828	O5*	G	D1054	-0.993	13.484	-58.088	1.00 55.82	RNA2 O
ATOM	2829	C5*	G	D1054	-2.203	13.659	-58.842	1.00 63.34	RNA2 C
ATOM	2830	C4*	G	D1054	-2.607	12.376	-59.540	1.00 61.66	RNA2 C
ATOM	2831	O4*	G	D1054	-1.612	11.993	-60.529	1.00 57.48	RNA2 O
ATOM	2832	C3*	G	D1054	-2.785	11.116	-58.707	1.00 58.52	RNA2 C
ATOM	2833	O3*	G	D1054	-4.027	11.063	-58.021	1.00 50.20	RNA2 O
ATOM	2834	C2*	G	D1054	-2.702	10.021	-59.766	1.00 54.72	RNA2 C
ATOM	2835	O2*	G	D1054	-3.915	9.849	-60.469	1.00 57.84	RNA2 O
ATOM	2836	C1*	G	D1054	-1.657	10.588	-60.723	1.00 42.15	RNA2 C
ATOM	2837	N9	G	D1054	-0.347	10.004	-60.453	1.00 43.98	RNA2 N
ATOM	2838	C8	G	D1054	0.686	10.525	-59.707	1.00 48.29	RNA2 C
ATOM	2839	N7	G	D1054	1.715	9.721	-59.624	1.00 48.90	RNA2 N
ATOM	2840	C5	G	D1054	1.340	8.607	-60.367	1.00 43.87	RNA2 C
ATOM	2841	C6	G	D1054	2.037	7.396	-60.634	1.00 37.83	RNA2 C
ATOM	2842	O6	G	D1054	3.167	7.050	-60.252	1.00 35.95	RNA2 O
ATOM	2843	N1	G	D1054	1.279	6.539	-61.428	1.00 42.56	RNA2 N
ATOM	2844	C2	G	D1054	0.013	6.807	-61.901	1.00 45.28	RNA2 C
ATOM	2845	N2	G	D1054	-0.567	5.854	-62.647	1.00 42.14	RNA2 N
ATOM	2846	N3	G	D1054	-0.642	7.925	-61.659	1.00 40.97	RNA2 N
ATOM	2847	C4	G	D1054	0.074	8.774	-60.892	1.00 45.06	RNA2 C
ATOM	2848	P	G	D1055	-4.174	10.115	-56.729	1.00 60.11	RNA2 P
ATOM	2849	O1P	G	D1055	-3.012	10.347	-55.817	1.00 52.31	RNA2 O
ATOM	2850	O2P	G	D1055	-5.562	10.287	-56.226	1.00 45.31	RNA2 O
ATOM	2851	O5*	G	D1055	-4.016	8.633	-57.297	1.00 61.25	RNA2 O
ATOM	2852	C5*	G	D1055	-5.060	8.044	-58.084	1.00 49.39	RNA2 C
ATOM	2853	C4*	G	D1055	-4.631	6.705	-58.643	1.00 46.06	RNA2 C
ATOM	2854	O4*	G	D1055	-3.395	6.848	-59.392	1.00 46.04	RNA2 O
ATOM	2855	C3*	G	D1055	-4.322	5.571	-57.678	1.00 46.58	RNA2 C
ATOM	2856	O3*	G	D1055	-5.478	4.904	-57.197	1.00 44.61	RNA2 O
ATOM	2857	C2*	G	D1055	-3.512	4.627	-58.556	1.00 50.61	RNA2 C
ATOM	2858	O2*	G	D1055	-4.337	3.844	-59.397	1.00 57.17	RNA2 O
ATOM	2859	C1*	G	D1055	-2.719	5.604	-59.419	1.00 37.93	RNA2 C
ATOM	2860	N9	G	D1055	-1.364	5.764	-58.905	1.00 28.75	RNA2 N
ATOM	2861	C8	G	D1055	-0.813	6.849	-58.266	1.00 28.74	RNA2 C
ATOM	2862	N7	G	D1055	0.437	6.662	-57.928	1.00 31.82	RNA2 N
ATOM	2863	C5	G	D1055	0.725	5.377	-58.371	1.00 24.53	RNA2 C
ATOM	2864	C6	G	D1055	1.924	4.619	-58.293	1.00 28.90	RNA2 C
ATOM	2865	O6	G	D1055	3.010	4.943	-57.807	1.00 32.85	RNA2 O
ATOM	2866	N1	G	D1055	1.771	3.360	-58.862	1.00 26.15	RNA2 N
ATOM	2867	C2	G	D1055	0.615	2.884	-59.432	1.00 32.58	RNA2 C
ATOM	2868	N2	G	D1055	0.658	1.635	-59.922	1.00 28.69	RNA2 N
ATOM	2869	N3	G	D1055	-0.505	3.580	-59.514	1.00 26.67	RNA2 N
ATOM	2870	C4	G	D1055	-0.377	4.809	-58.971	1.00 28.85	RNA2 C
ATOM	2871	P	G	D1056	-5.427	4.178	-55.764	1.00 41.37	RNA2 P
ATOM	2872	O1P	G	D1056	-5.088	5.212	-54.752	1.00 49.91	RNA2 O

ATOM	2873	O2P	G	D1056	-6.660	3.370	-55.603	1.00	41.24	RNA2	O
ATOM	2874	O5*	G	D1056	-4.173	3.205	-55.857	1.00	31.72	RNA2	O
ATOM	2875	C5*	G	D1056	-4.288	1.915	-56.458	1.00	26.06	RNA2	C
ATOM	2876	C4*	G	D1056	-2.992	1.163	-56.310	1.00	30.23	RNA2	C
ATOM	2877	O4*	G	D1056	-1.926	1.929	-56.923	1.00	33.12	RNA2	O
ATOM	2878	C3*	G	D1056	-2.520	0.944	-54.886	1.00	25.25	RNA2	C
ATOM	2879	O3*	G	D1056	-3.091	-0.214	-54.323	1.00	32.82	RNA2	O
ATOM	2880	C2*	G	D1056	-1.015	0.792	-55.044	1.00	30.19	RNA2	C
ATOM	2881	O2*	G	D1056	-0.631	-0.515	-55.418	1.00	28.72	RNA2	O
ATOM	2882	C1*	G	D1056	-0.728	1.769	-56.181	1.00	29.85	RNA2	C
ATOM	2883	N9	G	D1056	-0.326	3.081	-55.682	1.00	33.20	RNA2	N
ATOM	2884	C8	G	D1056	-1.142	4.165	-55.453	1.00	31.51	RNA2	C
ATOM	2885	N7	G	D1056	-0.496	5.205	-55.003	1.00	40.50	RNA2	N
ATOM	2886	C5	G	D1056	0.825	4.784	-54.926	1.00	37.25	RNA2	C
ATOM	2887	C6	G	D1056	1.985	5.481	-54.505	1.00	45.50	RNA2	C
ATOM	2888	O6	G	D1056	2.078	6.654	-54.106	1.00	54.00	RNA2	O
ATOM	2889	N1	G	D1056	3.122	4.677	-54.584	1.00	42.27	RNA2	N
ATOM	2890	C2	G	D1056	3.138	3.372	-55.020	1.00	38.28	RNA2	C
ATOM	2891	N2	G	D1056	4.337	2.765	-55.040	1.00	33.41	RNA2	N
ATOM	2892	N3	G	D1056	2.060	2.712	-55.413	1.00	35.91	RNA2	N
ATOM	2893	C4	G	D1056	0.947	3.474	-55.341	1.00	31.74	RNA2	C
ATOM	2894	P	A	D1057	-3.445	-0.241	-52.765	1.00	34.80	RNA2	P
ATOM	2895	O1P	A	D1057	-2.899	-1.503	-52.213	1.00	40.31	RNA2	O
ATOM	2896	O2P	A	D1057	-3.058	1.055	-52.152	1.00	39.35	RNA2	O
ATOM	2897	O5*	A	D1057	-5.027	-0.331	-52.754	1.00	19.58	RNA2	O
ATOM	2898	C5*	A	D1057	-5.823	0.724	-53.304	1.00	24.68	RNA2	C
ATOM	2899	C4*	A	D1057	-6.915	0.144	-54.161	1.00	26.68	RNA2	C
ATOM	2900	O4*	A	D1057	-6.359	-0.301	-55.425	1.00	40.11	RNA2	O
ATOM	2901	C3*	A	D1057	-7.560	-1.100	-53.585	1.00	30.27	RNA2	C
ATOM	2902	O3*	A	D1057	-8.559	-0.816	-52.635	1.00	35.52	RNA2	O
ATOM	2903	C2*	A	D1057	-8.090	-1.811	-54.820	1.00	30.75	RNA2	C
ATOM	2904	O2*	A	D1057	-9.317	-1.270	-55.268	1.00	24.78	RNA2	O
ATOM	2905	C1*	A	D1057	-6.991	-1.506	-55.834	1.00	16.37	RNA2	C
ATOM	2906	N9	A	D1057	-5.973	-2.559	-55.883	1.00	21.50	RNA2	N
ATOM	2907	C8	A	D1057	-4.626	-2.445	-55.613	1.00	18.28	RNA2	C
ATOM	2908	N7	A	D1057	-3.962	-3.566	-55.754	1.00	23.67	RNA2	N
ATOM	2909	C5	A	D1057	-4.935	-4.484	-56.140	1.00	21.49	RNA2	C
ATOM	2910	C6	A	D1057	-4.872	-5.852	-56.447	1.00	17.73	RNA2	C
ATOM	2911	N6	A	D1057	-3.748	-6.569	-56.412	1.00	22.33	RNA2	N
ATOM	2912	N1	A	D1057	-6.019	-6.470	-56.797	1.00	29.29	RNA2	N
ATOM	2913	C2	A	D1057	-7.150	-5.753	-56.829	1.00	30.01	RNA2	C
ATOM	2914	N3	A	D1057	-7.337	-4.465	-56.559	1.00	24.69	RNA2	N
ATOM	2915	C4	A	D1057	-6.177	-3.879	-56.219	1.00	18.45	RNA2	C
ATOM	2916	P	U	D1058	-8.746	-1.807	-51.399	1.00	30.93	RNA2	P
ATOM	2917	O1P	U	D1058	-7.361	-2.213	-50.993	1.00	24.94	RNA2	O

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ATOM  2918 O2P  U D1058     -9.669  -1.203 -50.402  1.00 29.08      RNA2 O
ATOM  2919 O5*  U D1058     -9.464  -3.068 -52.042  1.00 30.31      RNA2 O
ATOM  2920 C5*  U D1058    -10.859  -3.043 -52.331  1.00 28.81      RNA2 C
ATOM  2921 C4*  U D1058    -11.349  -4.440 -52.592  1.00 31.83      RNA2 C
ATOM  2922 O4*  U D1058    -10.668  -4.953 -53.765  1.00 33.24      RNA2 O
ATOM  2923 C3*  U D1058    -11.031  -5.471 -51.520  1.00 33.13      RNA2 C
ATOM  2924 O3*  U D1058    -11.925  -5.479 -50.425  1.00 32.98      RNA2 O
ATOM  2925 C2*  U D1058    -11.084  -6.772 -52.299  1.00 29.12      RNA2 C
ATOM  2926 O2*  U D1058    -12.414  -7.204 -52.513  1.00 29.74      RNA2 O
ATOM  2927 C1*  U D1058    -10.455  -6.348 -53.622  1.00 26.32      RNA2 C
ATOM  2928 N1   U D1058     -9.008  -6.614 -53.638  1.00 21.34      RNA2 N
ATOM  2929 C2   U D1058     -8.608  -7.932 -53.803  1.00 24.87      RNA2 C
ATOM  2930 O2   U D1058     -9.402  -8.853 -53.938  1.00 31.94      RNA2 O
ATOM  2931 N3   U D1058     -7.253  -8.136 -53.799  1.00  8.92      RNA2 N
ATOM  2932 C4   U D1058     -6.273  -7.188 -53.647  1.00 22.44      RNA2 C
ATOM  2933 O4   U D1058     -5.088  -7.533 -53.685  1.00 18.08      RNA2 O
ATOM  2934 C5   U D1058     -6.759  -5.848 -53.482  1.00 22.73      RNA2 C
ATOM  2935 C6   U D1058     -8.080  -5.614 -53.488  1.00 18.95      RNA2 C
ATOM  2936 P    G D1059    -11.432  -6.089 -49.022  1.00 29.43      RNA2 P
ATOM  2937 O1P  G D1059     -9.995  -5.757 -48.812  1.00 18.78      RNA2 O
ATOM  2938 O2P  G D1059    -12.431  -5.724 -47.993  1.00 38.92      RNA2 O
ATOM  2939 O5*  G D1059    -11.490  -7.659 -49.247  1.00 34.42      RNA2 O
ATOM  2940 C5*  G D1059    -12.729  -8.312 -49.534  1.00 29.33      RNA2 C
ATOM  2941 C4*  G D1059    -12.525  -9.801 -49.573  1.00 27.67      RNA2 C
ATOM  2942 O4*  G D1059    -11.608 -10.126 -50.645  1.00 28.30      RNA2 O
ATOM  2943 C3*  G D1059    -11.883 -10.411 -48.339  1.00 32.02      RNA2 C
ATOM  2944 O3*  G D1059    -12.840 -10.666 -47.314  1.00 37.54      RNA2 O
ATOM  2945 C2*  G D1059    -11.260 -11.691 -48.887  1.00 27.34      RNA2 C
ATOM  2946 O2*  G D1059    -12.207 -12.736 -48.993  1.00 21.26      RNA2 O
ATOM  2947 C1*  G D1059    -10.838 -11.258 -50.289  1.00 18.26      RNA2 C
ATOM  2948 N9   G D1059     -9.425 -10.920 -50.414  1.00 11.76      RNA2 N
ATOM  2949 C8   G D1059     -8.846  -9.686 -50.262  1.00 10.37      RNA2 C
ATOM  2950 N7   G D1059     -7.552  -9.700 -50.455  1.00 15.12      RNA2 N
ATOM  2951 C5   G D1059     -7.260 -11.026 -50.747  1.00  5.51      RNA2 C
ATOM  2952 C6   G D1059     -6.022 -11.652 -51.055  1.00 15.78      RNA2 C
ATOM  2953 O6   G D1059     -4.892 -11.145 -51.124  1.00 17.40      RNA2 O
ATOM  2954 N1   G D1059     -6.184 -13.009 -51.300  1.00 12.54      RNA2 N
ATOM  2955 C2   G D1059     -7.377 -13.685 -51.256  1.00 23.87      RNA2 C
ATOM  2956 N2   G D1059     -7.326 -14.997 -51.540  1.00 21.07      RNA2 N
ATOM  2957 N3   G D1059     -8.536 -13.119 -50.962  1.00 20.56      RNA2 N
ATOM  2958 C4   G D1059     -8.404 -11.794 -50.723  1.00 17.53      RNA2 C
ATOM  2959 P    U D1060    -12.363 -10.713 -45.780  1.00 31.30      RNA2 P
ATOM  2960 O1P  U D1060    -13.473 -10.167 -44.963  1.00 29.83      RNA2 O
ATOM  2961 O2P  U D1060    -11.840 -12.074 -45.484  1.00 37.29      RNA2 O
ATOM  2962 O5*  U D1060    -11.129  -9.708 -45.745  1.00 25.29      RNA2 O
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ATOM 2963 C5* U D1060 -10.735 -9.064 -44.527 1.00 22.54 RNA2 C
ATOM 2964 C4* U D1060 -9.378 -8.435 -44.692 1.00 22.65 RNA2 C
ATOM 2965 O4* U D1060 -8.401 -9.481 -44.882 1.00 24.56 RNA2 O
ATOM 2966 C3* U D1060 -9.238 -7.481 -45.870 1.00 26.03 RNA2 C
ATOM 2967 O3* U D1060 -8.303 -6.454 -45.522 1.00 41.53 RNA2 O
ATOM 2968 C2* U D1060 -8.608 -8.361 -46.946 1.00 31.11 RNA2 C
ATOM 2969 O2* U D1060 -7.808 -7.616 -47.841 1.00 45.38 RNA2 O
ATOM 2970 C1* U D1060 -7.735 -9.299 -46.110 1.00 26.61 RNA2 C
ATOM 2971 N1 U D1060 -7.519 -10.632 -46.690 1.00 21.85 RNA2 N
ATOM 2972 C2 U D1060 -6.291 -10.898 -47.261 1.00 23.55 RNA2 C
ATOM 2973 O2 U D1060 -5.402 -10.063 -47.355 1.00 21.48 RNA2 O
ATOM 2974 N3 U D1060 -6.141 -12.182 -47.726 1.00 25.97 RNA2 N
ATOM 2975 C4 U D1060 -7.076 -13.199 -47.691 1.00 28.32 RNA2 C
ATOM 2976 O4 U D1060 -6.778 -14.311 -48.139 1.00 27.53 RNA2 O
ATOM 2977 C5 U D1060 -8.329 -12.837 -47.107 1.00 18.41 RNA2 C
ATOM 2978 C6 U D1060 -8.507 -11.600 -46.642 1.00 21.87 RNA2 C
ATOM 2979 P U D1061 -8.630 -5.419 -44.325 1.00 28.91 RNA2 P
ATOM 2980 O1P U D1061 -8.173 -4.091 -44.810 1.00 33.68 RNA2 O
ATOM 2981 O2P U D1061 -10.037 -5.590 -43.863 1.00 15.62 RNA2 O
ATOM 2982 O5* U D1061 -7.649 -5.888 -43.161 1.00 19.70 RNA2 O
ATOM 2983 C5* U D1061 -6.225 -5.745 -43.301 1.00 18.21 RNA2 C
ATOM 2984 C4* U D1061 -5.514 -6.526 -42.225 1.00 27.99 RNA2 C
ATOM 2985 O4* U D1061 -5.894 -5.996 -40.927 1.00 36.85 RNA2 O
ATOM 2986 C3* U D1061 -5.800 -8.028 -42.181 1.00 29.80 RNA2 C
ATOM 2987 O3* U D1061 -4.608 -8.696 -41.772 1.00 33.59 RNA2 O
ATOM 2988 C2* U D1061 -6.812 -8.151 -41.043 1.00 33.22 RNA2 C
ATOM 2989 O2* U D1061 -6.748 -9.417 -40.415 1.00 27.78 RNA2 O
ATOM 2990 C1* U D1061 -6.313 -7.055 -40.102 1.00 42.74 RNA2 C
ATOM 2991 N1 U D1061 -7.205 -6.543 -39.046 1.00 44.96 RNA2 N
ATOM 2992 C2 U D1061 -6.737 -6.649 -37.742 1.00 53.51 RNA2 C
ATOM 2993 O2 U D1061 -5.650 -7.143 -37.464 1.00 44.65 RNA2 O
ATOM 2994 N3 U D1061 -7.579 -6.157 -36.776 1.00 60.76 RNA2 N
ATOM 2995 C4 U D1061 -8.811 -5.585 -36.961 1.00 51.80 RNA2 C
ATOM 2996 O4 U D1061 -9.435 -5.195 -35.977 1.00 48.61 RNA2 O
ATOM 2997 C5 U D1061 -9.240 -5.508 -38.333 1.00 40.80 RNA2 C
ATOM 2998 C6 U D1061 -8.440 -5.979 -39.307 1.00 43.37 RNA2 C
ATOM 2999 P G D1062 -3.700 -9.466 -42.848 1.00 33.56 RNA2 P
ATOM 3000 O1P G D1062 -3.835 -8.777 -44.158 1.00 35.31 RNA2 O
ATOM 3001 O2P G D1062 -2.353 -9.644 -42.252 1.00 21.04 RNA2 O
ATOM 3002 O5* G D1062 -4.367 -10.905 -42.956 1.00 30.74 RNA2 O
ATOM 3003 C5* G D1062 -5.563 -11.128 -43.737 1.00 36.95 RNA2 C
ATOM 3004 C4* G D1062 -5.583 -12.554 -44.235 1.00 30.45 RNA2 C
ATOM 3005 O4* G D1062 -4.531 -12.739 -45.222 1.00 26.47 RNA2 O
ATOM 3006 C3* G D1062 -5.264 -13.550 -43.139 1.00 20.89 RNA2 C
ATOM 3007 O3* G D1062 -6.428 -13.905 -42.431 1.00 31.67 RNA2 O

ATOM 3008 C2* G D1062 -4.625 -14.707 -43.894 1.00 23.56 RNA2 C
ATOM 3009 O2* G D1062 -5.589 -15.567 -44.466 1.00 18.76 RNA2 O
ATOM 3010 C1* G D1062 -3.854 -13.963 -44.988 1.00 16.90 RNA2 C
ATOM 3011 N9 G D1062 -2.473 -13.642 -44.620 1.00 13.03 RNA2 N
ATOM 3012 C8 G D1062 -1.919 -12.387 -44.523 1.00 19.49 RNA2 C
ATOM 3013 N7 G D1062 -0.660 -12.404 -44.173 1.00 13.70 RNA2 N
ATOM 3014 C5 G D1062 -0.362 -13.749 -44.024 1.00 14.04 RNA2 C
ATOM 3015 C6 G D1062 0.850 -14.379 -43.651 1.00 24.18 RNA2 C
ATOM 3016 O6 G D1062 1.933 -13.852 -43.356 1.00 29.04 RNA2 O
ATOM 3017 N1 G D1062 0.723 -15.765 -43.634 1.00 22.87 RNA2 N
ATOM 3018 C2 G D1062 -0.427 -16.456 -43.927 1.00 30.15 RNA2 C
ATOM 3019 N2 G D1062 -0.349 -17.795 -43.849 1.00 24.93 RNA2 N
ATOM 3020 N3 G D1062 -1.570 -15.878 -44.269 1.00 30.88 RNA2 N
ATOM 3021 C4 G D1062 -1.466 -14.531 -44.300 1.00 16.88 RNA2 C
ATOM 3022 P G D1063 -6.322 -14.242 -40.874 1.00 28.41 RNA2 P
ATOM 3023 O1P G D1063 -5.463 -13.199 -40.266 1.00 27.32 RNA2 O
ATOM 3024 O2P G D1063 -7.701 -14.468 -40.367 1.00 29.73 RNA2 O
ATOM 3025 O5* G D1063 -5.523 -15.617 -40.821 1.00 30.17 RNA2 O
ATOM 3026 C5* G D1063 -6.184 -16.864 -41.087 1.00 24.95 RNA2 C
ATOM 3027 C4* G D1063 -5.241 -18.011 -40.832 1.00 20.87 RNA2 C
ATOM 3028 O4* G D1063 -4.075 -17.850 -41.677 1.00 27.19 RNA2 O
ATOM 3029 C3* G D1063 -4.659 -18.092 -39.434 1.00 26.89 RNA2 C
ATOM 3030 O3* G D1063 -5.539 -18.706 -38.508 1.00 40.50 RNA2 O
ATOM 3031 C2* G D1063 -3.373 -18.869 -39.659 1.00 23.40 RNA2 C
ATOM 3032 O2* G D1063 -3.601 -20.256 -39.810 1.00 29.18 RNA2 O
ATOM 3033 C1* G D1063 -2.919 -18.297 -40.994 1.00 21.30 RNA2 C
ATOM 3034 N9 G D1063 -2.022 -17.158 -40.820 1.00 18.48 RNA2 N
ATOM 3035 C8 G D1063 -2.309 -15.827 -41.016 1.00 13.94 RNA2 C
ATOM 3036 N7 G D1063 -1.283 -15.044 -40.798 1.00 19.66 RNA2 N
ATOM 3037 C5 G D1063 -0.260 -15.909 -40.428 1.00 17.05 RNA2 C
ATOM 3038 C6 G D1063 1.093 -15.646 -40.066 1.00 24.81 RNA2 C
ATOM 3039 O6 G D1063 1.680 -14.559 -39.999 1.00 27.63 RNA2 O
ATOM 3040 N1 G D1063 1.776 -16.819 -39.756 1.00 29.06 RNA2 N
ATOM 3041 C2 G D1063 1.234 -18.080 -39.781 1.00 24.76 RNA2 C
ATOM 3042 N2 G D1063 2.051 -19.081 -39.433 1.00 26.32 RNA2 N
ATOM 3043 N3 G D1063 -0.018 -18.340 -40.119 1.00 25.89 RNA2 N
ATOM 3044 C4 G D1063 -0.702 -17.217 -40.429 1.00 24.85 RNA2 C
ATOM 3045 P C D1064 -5.606 -18.145 -37.003 1.00 33.12 RNA2 P
ATOM 3046 O1P C D1064 -5.740 -16.669 -37.090 1.00 33.72 RNA2 O
ATOM 3047 O2P C D1064 -6.628 -18.934 -36.261 1.00 34.10 RNA2 O
ATOM 3048 O5* C D1064 -4.159 -18.476 -36.424 1.00 27.13 RNA2 O
ATOM 3049 C5* C D1064 -3.695 -19.826 -36.395 1.00 16.79 RNA2 C
ATOM 3050 C4* C D1064 -2.235 -19.884 -36.032 1.00 25.70 RNA2 C
ATOM 3051 O4* C D1064 -1.436 -19.190 -37.022 1.00 29.89 RNA2 O
ATOM 3052 C3* C D1064 -1.813 -19.250 -34.720 1.00 29.70 RNA2 C

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ATOM  3053  O3*  C D1064     -2.095 -20.085 -33.611  1.00 37.04      RNA2 O
ATOM  3054  C2*  C D1064     -0.315 -19.047 -34.923  1.00 30.06      RNA2 C
ATOM  3055  O2*  C D1064      0.445 -20.216 -34.696  1.00 28.38      RNA2 O
ATOM  3056  C1*  C D1064     -0.251 -18.704 -36.409  1.00 30.33      RNA2 C
ATOM  3057  N1   C D1064     -0.140 -17.251 -36.627  1.00 20.71      RNA2 N
ATOM  3058  C2   C D1064      1.114 -16.655 -36.474  1.00 24.44      RNA2 C
ATOM  3059  O2   C D1064      2.086 -17.365 -36.175  1.00 30.49      RNA2 O
ATOM  3060  N3   C D1064      1.237 -15.325 -36.654  1.00 26.69      RNA2 N
ATOM  3061  C4   C D1064      0.170 -14.591 -36.976  1.00 20.50      RNA2 C
ATOM  3062  N4   C D1064      0.347 -13.279 -37.141  1.00 22.60      RNA2 N
ATOM  3063  C5   C D1064     -1.120 -15.169 -37.143  1.00 10.11      RNA2 C
ATOM  3064  C6   C D1064     -1.229 -16.492 -36.962  1.00 23.85      RNA2 C
ATOM  3065  P    U D1065     -2.513 -19.420 -32.214  1.00 35.56      RNA2 P
ATOM  3066  O1P  U D1065     -3.615 -18.460 -32.467  1.00 26.06      RNA2 O
ATOM  3067  O2P  U D1065     -2.716 -20.527 -31.248  1.00 43.50      RNA2 O
ATOM  3068  O5*  U D1065     -1.209 -18.600 -31.807  1.00 27.70      RNA2 O
ATOM  3069  C5*  U D1065      0.044 -19.282 -31.609  1.00 30.92      RNA2 C
ATOM  3070  C4*  U D1065      1.168 -18.287 -31.469  1.00 30.67      RNA2 C
ATOM  3071  O4*  U D1065      1.332 -17.559 -32.713  1.00 39.57      RNA2 O
ATOM  3072  C3*  U D1065      0.951 -17.209 -30.423  1.00 36.18      RNA2 C
ATOM  3073  O3*  U D1065      1.285 -17.667 -29.123  1.00 36.24      RNA2 O
ATOM  3074  C2*  U D1065      1.843 -16.076 -30.921  1.00 38.21      RNA2 C
ATOM  3075  O2*  U D1065      3.207 -16.224 -30.578  1.00 34.14      RNA2 O
ATOM  3076  C1*  U D1065      1.692 -16.216 -32.437  1.00 34.96      RNA2 C
ATOM  3077  N1   U D1065      0.645 -15.327 -32.968  1.00 22.93      RNA2 N
ATOM  3078  C2   U D1065      1.028 -14.066 -33.377  1.00 24.04      RNA2 C
ATOM  3079  O2   U D1065      2.187 -13.674 -33.325  1.00 20.47      RNA2 O
ATOM  3080  N3   U D1065      0.008 -13.276 -33.849  1.00 17.91      RNA2 N
ATOM  3081  C4   U D1065     -1.325 -13.612 -33.954  1.00 25.02      RNA2 C
ATOM  3082  O4   U D1065     -2.125 -12.793 -34.424  1.00 30.88      RNA2 O
ATOM  3083  C5   U D1065     -1.640 -14.934 -33.511  1.00 26.71      RNA2 C
ATOM  3084  C6   U D1065     -0.670 -15.727 -33.046  1.00 28.23      RNA2 C
ATOM  3085  P    U D1066      0.342 -17.279 -27.876  1.00 35.54      RNA2 P
ATOM  3086  O1P  U D1066     -1.089 -17.498 -28.212  1.00 19.51      RNA2 O
ATOM  3087  O2P  U D1066      0.927 -17.960 -26.692  1.00 43.24      RNA2 O
ATOM  3088  O5*  U D1066      0.552 -15.708 -27.728  1.00 32.79      RNA2 O
ATOM  3089  C5*  U D1066      1.867 -15.163 -27.509  1.00 39.57      RNA2 C
ATOM  3090  C4*  U D1066      1.853 -13.664 -27.695  1.00 41.26      RNA2 C
ATOM  3091  O4*  U D1066      1.606 -13.339 -29.088  1.00 50.01      RNA2 O
ATOM  3092  C3*  U D1066      0.773 -12.909 -26.935  1.00 46.81      RNA2 C
ATOM  3093  O3*  U D1066      1.137 -12.653 -25.587  1.00 47.16      RNA2 O
ATOM  3094  C2*  U D1066      0.645 -11.626 -27.743  1.00 45.38      RNA2 C
ATOM  3095  O2*  U D1066      1.671 -10.702 -27.422  1.00 47.24      RNA2 O
ATOM  3096  C1*  U D1066      0.848 -12.142 -29.168  1.00 44.66      RNA2 C
ATOM  3097  N1   U D1066     -0.437 -12.423 -29.835  1.00 36.02      RNA2 N
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ATOM	3098	C2	U D1066	-1.001	-11.401	-30.583	1.00	31.01	RNA2 C
ATOM	3099	O2	U D1066	-0.450	-10.325	-30.752	1.00	24.12	RNA2 O
ATOM	3100	N3	U D1066	-2.231	-11.687	-31.131	1.00	26.04	RNA2 N
ATOM	3101	C4	U D1066	-2.939	-12.872	-31.028	1.00	32.10	RNA2 C
ATOM	3102	O4	U D1066	-4.082	-12.941	-31.501	1.00	32.26	RNA2 O
ATOM	3103	C5	U D1066	-2.276	-13.895	-30.271	1.00	27.27	RNA2 C
ATOM	3104	C6	U D1066	-1.080	-13.644	-29.712	1.00	35.51	RNA2 C
ATOM	3105	P	A D1067	0.011	-12.695	-24.442	1.00	41.56	RNA2 P
ATOM	3106	O1P	A D1067	-0.869	-13.868	-24.667	1.00	35.90	RNA2 O
ATOM	3107	O2P	A D1067	0.710	-12.532	-23.138	1.00	61.37	RNA2 O
ATOM	3108	O5*	A D1067	-0.877	-11.403	-24.702	1.00	37.80	RNA2 O
ATOM	3109	C5*	A D1067	-2.175	-11.275	-24.099	1.00	33.78	RNA2 C
ATOM	3110	C4*	A D1067	-2.689	-9.870	-24.284	1.00	40.27	RNA2 C
ATOM	3111	O4*	A D1067	-1.791	-8.952	-23.617	1.00	40.68	RNA2 O
ATOM	3112	C3*	A D1067	-2.714	-9.402	-25.727	1.00	40.11	RNA2 C
ATOM	3113	O3*	A D1067	-3.918	-9.794	-26.362	1.00	46.79	RNA2 O
ATOM	3114	C2*	A D1067	-2.560	-7.892	-25.606	1.00	33.18	RNA2 C
ATOM	3115	O2*	A D1067	-3.785	-7.245	-25.315	1.00	34.55	RNA2 O
ATOM	3116	C1*	A D1067	-1.637	-7.782	-24.394	1.00	30.38	RNA2 C
ATOM	3117	N9	A D1067	-0.216	-7.636	-24.699	1.00	18.52	RNA2 N
ATOM	3118	C8	A D1067	0.791	-8.539	-24.462	1.00	19.03	RNA2 C
ATOM	3119	N7	A D1067	1.987	-8.090	-24.769	1.00	23.17	RNA2 N
ATOM	3120	C5	A D1067	1.748	-6.814	-25.262	1.00	12.64	RNA2 C
ATOM	3121	C6	A D1067	2.605	-5.811	-25.748	1.00	16.33	RNA2 C
ATOM	3122	N6	A D1067	3.934	-5.945	-25.831	1.00	21.10	RNA2 N
ATOM	3123	N1	A D1067	2.046	-4.651	-26.154	1.00	17.93	RNA2 N
ATOM	3124	C2	A D1067	0.714	-4.518	-26.077	1.00	24.51	RNA2 C
ATOM	3125	N3	A D1067	-0.197	-5.388	-25.642	1.00	23.41	RNA2 N
ATOM	3126	C4	A D1067	0.393	-6.528	-25.240	1.00	22.32	RNA2 C
ATOM	3127	P	G D1068	-3.863	-10.352	-27.861	1.00	37.45	RNA2 P
ATOM	3128	O1P	G D1068	-2.775	-11.365	-27.915	1.00	32.87	RNA2 O
ATOM	3129	O2P	G D1068	-5.247	-10.719	-28.265	1.00	30.61	RNA2 O
ATOM	3130	O5*	G D1068	-3.399	-9.084	-28.697	1.00	34.59	RNA2 O
ATOM	3131	C5*	G D1068	-4.254	-7.938	-28.794	1.00	32.91	RNA2 C
ATOM	3132	C4*	G D1068	-3.550	-6.828	-29.521	1.00	39.65	RNA2 C
ATOM	3133	O4*	G D1068	-2.460	-6.334	-28.708	1.00	34.36	RNA2 O
ATOM	3134	C3*	G D1068	-2.908	-7.218	-30.840	1.00	41.96	RNA2 C
ATOM	3135	O3*	G D1068	-3.874	-7.194	-31.893	1.00	38.73	RNA2 O
ATOM	3136	C2*	G D1068	-1.811	-6.168	-30.989	1.00	37.55	RNA2 C
ATOM	3137	O2*	G D1068	-2.315	-4.944	-31.487	1.00	54.39	RNA2 O
ATOM	3138	C1*	G D1068	-1.382	-5.951	-29.535	1.00	22.83	RNA2 C
ATOM	3139	N9	G D1068	-0.226	-6.739	-29.134	1.00	20.42	RNA2 N
ATOM	3140	C8	G D1068	-0.246	-8.011	-28.616	1.00	22.08	RNA2 C
ATOM	3141	N7	G D1068	0.944	-8.464	-28.328	1.00	22.50	RNA2 N
ATOM	3142	C5	G D1068	1.803	-7.433	-28.683	1.00	10.90	RNA2 C

ATOM	3143	C6	G	D1068	3.211	-7.347	-28.595	1.00	18.64	RNA2	C
ATOM	3144	O6	G	D1068	4.011	-8.196	-28.176	1.00	32.91	RNA2	O
ATOM	3145	N1	G	D1068	3.679	-6.123	-29.060	1.00	12.16	RNA2	N
ATOM	3146	C2	G	D1068	2.894	-5.115	-29.547	1.00	13.74	RNA2	C
ATOM	3147	N2	G	D1068	3.543	-4.013	-29.960	1.00	20.53	RNA2	N
ATOM	3148	N3	G	D1068	1.575	-5.179	-29.629	1.00	16.63	RNA2	N
ATOM	3149	C4	G	D1068	1.100	-6.360	-29.184	1.00	16.14	RNA2	C
ATOM	3150	P	A	D1069	-3.995	-8.447	-32.902	1.00	27.21	RNA2	P
ATOM	3151	O1P	A	D1069	-4.082	-9.718	-32.124	1.00	34.28	RNA2	O
ATOM	3152	O2P	A	D1069	-5.070	-8.102	-33.864	1.00	29.02	RNA2	O
ATOM	3153	O5*	A	D1069	-2.601	-8.445	-33.661	1.00	13.61	RNA2	O
ATOM	3154	C5*	A	D1069	-2.231	-7.337	-34.472	1.00	12.04	RNA2	C
ATOM	3155	C4*	A	D1069	-0.867	-7.557	-35.055	1.00	21.87	RNA2	C
ATOM	3156	O4*	A	D1069	0.149	-7.322	-34.046	1.00	32.63	RNA2	O
ATOM	3157	C3*	A	D1069	-0.590	-8.954	-35.628	1.00	35.90	RNA2	C
ATOM	3158	O3*	A	D1069	0.162	-8.819	-36.833	1.00	43.63	RNA2	O
ATOM	3159	C2*	A	D1069	0.352	-9.560	-34.592	1.00	35.57	RNA2	C
ATOM	3160	O2*	A	D1069	1.241	-10.526	-35.127	1.00	44.23	RNA2	O
ATOM	3161	C1*	A	D1069	1.127	-8.311	-34.199	1.00	42.00	RNA2	C
ATOM	3162	N9	A	D1069	2.031	-8.358	-33.054	1.00	38.32	RNA2	N
ATOM	3163	C8	A	D1069	2.071	-9.207	-31.976	1.00	30.76	RNA2	C
ATOM	3164	N7	A	D1069	3.141	-9.059	-31.233	1.00	35.91	RNA2	N
ATOM	3165	C5	A	D1069	3.827	-8.017	-31.841	1.00	33.30	RNA2	C
ATOM	3166	C6	A	D1069	5.053	-7.392	-31.552	1.00	39.74	RNA2	C
ATOM	3167	N6	A	D1069	5.850	-7.751	-30.540	1.00	50.68	RNA2	N
ATOM	3168	N1	A	D1069	5.443	-6.375	-32.353	1.00	41.06	RNA2	N
ATOM	3169	C2	A	D1069	4.649	-6.022	-33.371	1.00	43.25	RNA2	C
ATOM	3170	N3	A	D1069	3.483	-6.540	-33.747	1.00	36.03	RNA2	N
ATOM	3171	C4	A	D1069	3.131	-7.548	-32.935	1.00	31.57	RNA2	C
ATOM	3172	P	A	D1070	-0.353	-9.514	-38.183	1.00	39.29	RNA2	P
ATOM	3173	O1P	A	D1070	0.847	-9.589	-39.057	1.00	23.58	RNA2	O
ATOM	3174	O2P	A	D1070	-1.128	-10.747	-37.873	1.00	27.46	RNA2	O
ATOM	3175	O5*	A	D1070	-1.376	-8.452	-38.783	1.00	32.87	RNA2	O
ATOM	3176	C5*	A	D1070	-0.906	-7.233	-39.388	1.00	32.49	RNA2	C
ATOM	3177	C4*	A	D1070	-2.018	-6.594	-40.179	1.00	35.94	RNA2	C
ATOM	3178	O4*	A	D1070	-3.134	-6.304	-39.296	1.00	34.73	RNA2	O
ATOM	3179	C3*	A	D1070	-1.665	-5.292	-40.885	1.00	39.27	RNA2	C
ATOM	3180	O3*	A	D1070	-2.329	-5.275	-42.147	1.00	42.75	RNA2	O
ATOM	3181	C2*	A	D1070	-2.248	-4.225	-39.960	1.00	39.48	RNA2	C
ATOM	3182	O2*	A	D1070	-2.656	-3.052	-40.635	1.00	46.91	RNA2	O
ATOM	3183	C1*	A	D1070	-3.468	-4.935	-39.379	1.00	38.47	RNA2	C
ATOM	3184	N9	A	D1070	-3.821	-4.467	-38.038	1.00	42.60	RNA2	N
ATOM	3185	C8	A	D1070	-3.112	-4.646	-36.878	1.00	43.81	RNA2	C
ATOM	3186	N7	A	D1070	-3.690	-4.133	-35.822	1.00	45.93	RNA2	N
ATOM	3187	C5	A	D1070	-4.854	-3.570	-36.318	1.00	44.50	RNA2	C

ATOM	3188	C6	A	D1070	-5.898	-2.873	-35.697	1.00 50.91	RNA2 C
ATOM	3189	N6	A	D1070	-5.936	-2.617	-34.390	1.00 62.29	RNA2 N
ATOM	3190	N1	A	D1070	-6.915	-2.441	-36.474	1.00 49.05	RNA2 N
ATOM	3191	C2	A	D1070	-6.870	-2.698	-37.783	1.00 37.67	RNA2 C
ATOM	3192	N3	A	D1070	-5.940	-3.344	-38.485	1.00 40.26	RNA2 N
ATOM	3193	C4	A	D1070	-4.946	-3.761	-37.683	1.00 42.22	RNA2 C
ATOM	3194	P	G	D1071	-1.684	-4.476	-43.382	1.00 30.55	RNA2 P
ATOM	3195	O1P	G	D1071	-2.623	-4.642	-44.520	1.00 33.24	RNA2 O
ATOM	3196	O2P	G	D1071	-1.310	-3.114	-42.932	1.00 42.96	RNA2 O
ATOM	3197	O5*	G	D1071	-0.331	-5.246	-43.697	1.00 21.65	RNA2 O
ATOM	3198	C5*	G	D1071	-0.333	-6.592	-44.214	1.00 29.38	RNA2 C
ATOM	3199	C4*	G	D1071	1.026	-6.907	-44.779	1.00 23.80	RNA2 C
ATOM	3200	O4*	G	D1071	1.238	-6.061	-45.928	1.00 28.20	RNA2 O
ATOM	3201	C3*	G	D1071	2.141	-6.557	-43.811	1.00 30.81	RNA2 C
ATOM	3202	O3*	G	D1071	2.441	-7.666	-42.979	1.00 41.31	RNA2 O
ATOM	3203	C2*	G	D1071	3.288	-6.132	-44.719	1.00 22.22	RNA2 C
ATOM	3204	O2*	G	D1071	4.080	-7.199	-45.191	1.00 28.60	RNA2 O
ATOM	3205	C1*	G	D1071	2.532	-5.498	-45.883	1.00 21.88	RNA2 C
ATOM	3206	N9	G	D1071	2.369	-4.053	-45.773	1.00 20.68	RNA2 N
ATOM	3207	C8	G	D1071	1.186	-3.366	-45.636	1.00 17.70	RNA2 C
ATOM	3208	N7	G	D1071	1.347	-2.072	-45.623	1.00 24.21	RNA2 N
ATOM	3209	C5	G	D1071	2.716	-1.895	-45.742	1.00 13.42	RNA2 C
ATOM	3210	C6	G	D1071	3.478	-0.710	-45.794	1.00 24.45	RNA2 C
ATOM	3211	O6	G	D1071	3.078	0.460	-45.758	1.00 34.15	RNA2 O
ATOM	3212	N1	G	D1071	4.841	-0.981	-45.904	1.00 15.33	RNA2 N
ATOM	3213	C2	G	D1071	5.395	-2.241	-45.961	1.00 23.28	RNA2 C
ATOM	3214	N2	G	D1071	6.734	-2.306	-46.052	1.00 12.46	RNA2 N
ATOM	3215	N3	G	D1071	4.686	-3.356	-45.925	1.00 19.68	RNA2 N
ATOM	3216	C4	G	D1071	3.363	-3.109	-45.817	1.00 12.68	RNA2 C
ATOM	3217	P	C	D1072	2.695	-7.430	-41.419	1.00 33.36	RNA2 P
ATOM	3218	O1P	C	D1072	1.653	-6.490	-40.920	1.00 33.81	RNA2 O
ATOM	3219	O2P	C	D1072	2.864	-8.759	-40.777	1.00 35.75	RNA2 O
ATOM	3220	O5*	C	D1072	4.090	-6.677	-41.393	1.00 20.85	RNA2 O
ATOM	3221	C5*	C	D1072	5.294	-7.370	-41.724	1.00 18.04	RNA2 C
ATOM	3222	C4*	C	D1072	6.458	-6.420	-41.676	1.00 27.13	RNA2 C
ATOM	3223	O4*	C	D1072	6.309	-5.437	-42.729	1.00 37.39	RNA2 O
ATOM	3224	C3*	C	D1072	6.577	-5.591	-40.408	1.00 33.89	RNA2 C
ATOM	3225	O3*	C	D1072	7.216	-6.295	-39.352	1.00 27.21	RNA2 O
ATOM	3226	C2*	C	D1072	7.364	-4.376	-40.882	1.00 36.24	RNA2 C
ATOM	3227	O2*	C	D1072	8.753	-4.637	-40.967	1.00 40.82	RNA2 O
ATOM	3228	C1*	C	D1072	6.803	-4.182	-42.291	1.00 32.40	RNA2 C
ATOM	3229	N1	C	D1072	5.704	-3.196	-42.347	1.00 21.10	RNA2 N
ATOM	3230	C2	C	D1072	6.015	-1.860	-42.594	1.00 22.51	RNA2 C
ATOM	3231	O2	C	D1072	7.206	-1.541	-42.755	1.00 32.30	RNA2 O
ATOM	3232	N3	C	D1072	5.016	-0.947	-42.647	1.00 18.99	RNA2 N

ATOM	3233	C4	C	D1072	3.750	-1.327	-42.456	1.00	23.03	RNA2	C
ATOM	3234	N4	C	D1072	2.795	-0.389	-42.506	1.00	21.64	RNA2	N
ATOM	3235	C5	C	D1072	3.405	-2.681	-42.204	1.00	18.92	RNA2	C
ATOM	3236	C6	C	D1072	4.404	-3.575	-42.160	1.00	22.99	RNA2	C
ATOM	3237	P	A	D1073	6.502	-6.360	-37.915	1.00	37.37	RNA2	P
ATOM	3238	O1P	A	D1073	6.300	-4.954	-37.487	1.00	30.80	RNA2	O
ATOM	3239	O2P	A	D1073	5.328	-7.287	-37.972	1.00	26.29	RNA2	O
ATOM	3240	O5*	A	D1073	7.614	-6.996	-36.980	1.00	33.33	RNA2	O
ATOM	3241	C5*	A	D1073	8.842	-6.293	-36.711	1.00	45.87	RNA2	C
ATOM	3242	C4*	A	D1073	9.614	-7.024	-35.651	1.00	39.23	RNA2	C
ATOM	3243	O4*	A	D1073	8.804	-7.060	-34.451	1.00	42.33	RNA2	O
ATOM	3244	C3*	A	D1073	9.847	-8.484	-35.996	1.00	42.31	RNA2	C
ATOM	3245	O3*	A	D1073	11.022	-8.666	-36.753	1.00	46.57	RNA2	O
ATOM	3246	C2*	A	D1073	9.902	-9.161	-34.638	1.00	40.15	RNA2	C
ATOM	3247	O2*	A	D1073	11.169	-9.047	-34.018	1.00	50.42	RNA2	O
ATOM	3248	C1*	A	D1073	8.866	-8.350	-33.866	1.00	29.91	RNA2	C
ATOM	3249	N9	A	D1073	7.532	-8.935	-33.963	1.00	24.96	RNA2	N
ATOM	3250	C8	A	D1073	6.453	-8.438	-34.648	1.00	25.01	RNA2	C
ATOM	3251	N7	A	D1073	5.373	-9.170	-34.534	1.00	31.09	RNA2	N
ATOM	3252	C5	A	D1073	5.770	-10.224	-33.727	1.00	16.48	RNA2	C
ATOM	3253	C6	A	D1073	5.085	-11.338	-33.237	1.00	25.59	RNA2	C
ATOM	3254	N6	A	D1073	3.804	-11.589	-33.504	1.00	28.23	RNA2	N
ATOM	3255	N1	A	D1073	5.765	-12.201	-32.456	1.00	25.23	RNA2	N
ATOM	3256	C2	A	D1073	7.053	-11.951	-32.200	1.00	27.30	RNA2	C
ATOM	3257	N3	A	D1073	7.811	-10.937	-32.608	1.00	31.09	RNA2	N
ATOM	3258	C4	A	D1073	7.099	-10.097	-33.375	1.00	27.01	RNA2	C
ATOM	3259	P	G	D1074	11.030	-9.753	-37.924	1.00	43.98	RNA2	P
ATOM	3260	O1P	G	D1074	9.978	-9.343	-38.892	1.00	47.14	RNA2	O
ATOM	3261	O2P	G	D1074	12.435	-9.917	-38.384	1.00	36.10	RNA2	O
ATOM	3262	O5*	G	D1074	10.556	-11.084	-37.192	1.00	30.43	RNA2	O
ATOM	3263	C5*	G	D1074	11.408	-11.715	-36.230	1.00	29.08	RNA2	C
ATOM	3264	C4*	G	D1074	10.753	-12.951	-35.675	1.00	27.13	RNA2	C
ATOM	3265	O4*	G	D1074	9.559	-12.586	-34.940	1.00	25.79	RNA2	O
ATOM	3266	C3*	G	D1074	10.260	-13.964	-36.689	1.00	34.21	RNA2	C
ATOM	3267	O3*	G	D1074	11.289	-14.803	-37.175	1.00	42.20	RNA2	O
ATOM	3268	C2*	G	D1074	9.202	-14.730	-35.908	1.00	33.31	RNA2	C
ATOM	3269	O2*	G	D1074	9.747	-15.738	-35.080	1.00	37.22	RNA2	O
ATOM	3270	C1*	G	D1074	8.598	-13.621	-35.049	1.00	21.21	RNA2	C
ATOM	3271	N9	G	D1074	7.387	-13.070	-35.648	1.00	27.34	RNA2	N
ATOM	3272	C8	G	D1074	7.235	-11.852	-36.268	1.00	27.08	RNA2	C
ATOM	3273	N7	G	D1074	6.017	-11.640	-36.688	1.00	25.47	RNA2	N
ATOM	3274	C5	G	D1074	5.325	-12.787	-36.327	1.00	19.99	RNA2	C
ATOM	3275	C6	G	D1074	3.966	-13.130	-36.504	1.00	30.58	RNA2	C
ATOM	3276	O6	G	D1074	3.063	-12.460	-37.021	1.00	35.90	RNA2	O
ATOM	3277	N1	G	D1074	3.687	-14.396	-35.992	1.00	36.16	RNA2	N

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ATOM  3278  C2   G D1074     4.597 -15.219 -35.379  1.00 34.56      RNA2 C
ATOM  3279  N2   G D1074     4.134 -16.400 -34.936  1.00 34.63      RNA2 N
ATOM  3280  N3   G D1074     5.868 -14.906 -35.205  1.00 31.20      RNA2 N
ATOM  3281  C4   G D1074     6.159 -13.683 -35.695  1.00 23.24      RNA2 C
ATOM  3282  P    C D1075    11.130 -15.471 -38.624  1.00 45.43      RNA2 P
ATOM  3283  O1P  C D1075    10.527 -14.447 -39.520  1.00 54.70      RNA2 O
ATOM  3284  O2P  C D1075    12.430 -16.096 -38.995  1.00 41.18      RNA2 O
ATOM  3285  O5*  C D1075    10.046 -16.607 -38.379  1.00 33.77      RNA2 O
ATOM  3286  C5*  C D1075    10.384 -17.767 -37.609  1.00 31.73      RNA2 C
ATOM  3287  C4*  C D1075     9.233 -18.737 -37.587  1.00 31.50      RNA2 C
ATOM  3288  O4*  C D1075     8.122 -18.137 -36.879  1.00 31.95      RNA2 O
ATOM  3289  C3*  C D1075     8.653 -19.112 -38.940  1.00 34.59      RNA2 C
ATOM  3290  O3*  C D1075     9.390 -20.130 -39.596  1.00 42.98      RNA2 O
ATOM  3291  C2*  C D1075     7.239 -19.539 -38.581  1.00 30.88      RNA2 C
ATOM  3292  O2*  C D1075     7.175 -20.852 -38.064  1.00 24.97      RNA2 O
ATOM  3293  C1*  C D1075     6.902 -18.546 -37.472  1.00 31.01      RNA2 C
ATOM  3294  N1   C D1075     6.223 -17.355 -38.013  1.00 26.90      RNA2 N
ATOM  3295  C2   C D1075     4.831 -17.388 -38.173  1.00 32.07      RNA2 C
ATOM  3296  O2   C D1075     4.206 -18.407 -37.825  1.00 31.32      RNA2 O
ATOM  3297  N3   C D1075     4.204 -16.313 -38.700  1.00 31.52      RNA2 N
ATOM  3298  C4   C D1075     4.908 -15.237 -39.059  1.00 24.70      RNA2 C
ATOM  3299  N4   C D1075     4.246 -14.208 -39.592  1.00 23.21      RNA2 N
ATOM  3300  C5   C D1075     6.320 -15.169 -38.892  1.00 20.78      RNA2 C
ATOM  3301  C6   C D1075     6.932 -16.239 -38.370  1.00 26.55      RNA2 C
ATOM  3302  P    C D1076     9.458 -20.140 -41.200  1.00 41.54      RNA2 P
ATOM  3303  O1P  C D1076     9.719 -18.749 -41.663  1.00 42.90      RNA2 O
ATOM  3304  O2P  C D1076    10.363 -21.241 -41.628  1.00 43.49      RNA2 O
ATOM  3305  O5*  C D1076     7.973 -20.524 -41.614  1.00 36.12      RNA2 O
ATOM  3306  C5*  C D1076     7.448 -21.808 -41.272  1.00 35.93      RNA2 C
ATOM  3307  C4*  C D1076     6.024 -21.941 -41.742  1.00 36.70      RNA2 C
ATOM  3308  O4*  C D1076     5.179 -21.022 -41.003  1.00 41.67      RNA2 O
ATOM  3309  C3*  C D1076     5.735 -21.611 -43.198  1.00 33.47      RNA2 C
ATOM  3310  O3*  C D1076     6.076 -22.654 -44.099  1.00 41.74      RNA2 O
ATOM  3311  C2*  C D1076     4.240 -21.334 -43.160  1.00 38.53      RNA2 C
ATOM  3312  O2*  C D1076     3.483 -22.530 -43.103  1.00 31.60      RNA2 O
ATOM  3313  C1*  C D1076     4.107 -20.590 -41.831  1.00 39.34      RNA2 C
ATOM  3314  N1   C D1076     4.199 -19.124 -42.018  1.00 25.11      RNA2 N
ATOM  3315  C2   C D1076     3.048 -18.421 -42.397  1.00 28.28      RNA2 C
ATOM  3316  O2   C D1076     1.978 -19.045 -42.536  1.00 22.07      RNA2 O
ATOM  3317  N3   C D1076     3.127 -17.083 -42.605  1.00 27.17      RNA2 N
ATOM  3318  C4   C D1076     4.293 -16.452 -42.451  1.00 27.03      RNA2 C
ATOM  3319  N4   C D1076     4.330 -15.136 -42.681  1.00 24.90      RNA2 N
ATOM  3320  C5   C D1076     5.475 -17.140 -42.056  1.00 21.98      RNA2 C
ATOM  3321  C6   C D1076     5.384 -18.460 -41.849  1.00 26.59      RNA2 C
ATOM  3322  P    A D1077     6.603 -22.281 -45.575  1.00 39.40      RNA2 P
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ATOM	3323	O1P	A	D1077	7.618	-21.198	-45.455	1.00	25.39	RNA2	O
ATOM	3324	O2P	A	D1077	6.965	-23.549	-46.255	1.00	45.75	RNA2	O
ATOM	3325	O5*	A	D1077	5.308	-21.688	-46.290	1.00	35.32	RNA2	O
ATOM	3326	C5*	A	D1077	4.132	-22.496	-46.434	1.00	30.36	RNA2	C
ATOM	3327	C4*	A	D1077	2.948	-21.659	-46.863	1.00	39.87	RNA2	C
ATOM	3328	O4*	A	D1077	2.657	-20.660	-45.852	1.00	36.52	RNA2	O
ATOM	3329	C3*	A	D1077	3.067	-20.856	-48.149	1.00	35.06	RNA2	C
ATOM	3330	O3*	A	D1077	2.842	-21.640	-49.313	1.00	33.77	RNA2	O
ATOM	3331	C2*	A	D1077	1.981	-19.801	-47.965	1.00	41.16	RNA2	C
ATOM	3332	O2*	A	D1077	0.677	-20.271	-48.264	1.00	33.46	RNA2	O
ATOM	3333	C1*	A	D1077	2.078	-19.520	-46.466	1.00	37.76	RNA2	C
ATOM	3334	N9	A	D1077	2.924	-18.352	-46.211	1.00	25.78	RNA2	N
ATOM	3335	C8	A	D1077	4.243	-18.300	-45.836	1.00	18.19	RNA2	C
ATOM	3336	N7	A	D1077	4.722	-17.081	-45.756	1.00	17.18	RNA2	N
ATOM	3337	C5	A	D1077	3.639	-16.275	-46.087	1.00	18.35	RNA2	C
ATOM	3338	C6	A	D1077	3.492	-14.874	-46.208	1.00	24.31	RNA2	C
ATOM	3339	N6	A	D1077	4.486	-13.996	-46.008	1.00	25.10	RNA2	N
ATOM	3340	N1	A	D1077	2.277	-14.401	-46.558	1.00	22.28	RNA2	N
ATOM	3341	C2	A	D1077	1.285	-15.278	-46.776	1.00	17.11	RNA2	C
ATOM	3342	N3	A	D1077	1.302	-16.604	-46.702	1.00	22.31	RNA2	N
ATOM	3343	C4	A	D1077	2.522	-17.044	-46.352	1.00	17.88	RNA2	C
ATOM	3344	P	U	D1078	3.650	-21.306	-50.662	1.00	27.11	RNA2	P
ATOM	3345	O1P	U	D1078	5.104	-21.343	-50.374	1.00	20.77	RNA2	O
ATOM	3346	O2P	U	D1078	3.091	-22.176	-51.728	1.00	43.45	RNA2	O
ATOM	3347	O5*	U	D1078	3.288	-19.785	-50.981	1.00	30.32	RNA2	O
ATOM	3348	C5*	U	D1078	1.985	-19.408	-51.478	1.00	30.56	RNA2	C
ATOM	3349	C4*	U	D1078	1.896	-17.901	-51.631	1.00	32.53	RNA2	C
ATOM	3350	O4*	U	D1078	2.062	-17.283	-50.329	1.00	27.97	RNA2	O
ATOM	3351	C3*	U	D1078	2.967	-17.244	-52.497	1.00	36.01	RNA2	C
ATOM	3352	O3*	U	D1078	2.620	-17.183	-53.871	1.00	42.75	RNA2	O
ATOM	3353	C2*	U	D1078	2.990	-15.821	-51.961	1.00	36.74	RNA2	C
ATOM	3354	O2*	U	D1078	1.935	-15.045	-52.493	1.00	40.26	RNA2	O
ATOM	3355	C1*	U	D1078	2.744	-16.048	-50.472	1.00	35.91	RNA2	C
ATOM	3356	N1	U	D1078	4.015	-16.102	-49.729	1.00	25.89	RNA2	N
ATOM	3357	C2	U	D1078	4.637	-14.892	-49.423	1.00	35.33	RNA2	C
ATOM	3358	O2	U	D1078	4.167	-13.800	-49.730	1.00	30.93	RNA2	O
ATOM	3359	N3	U	D1078	5.830	-15.008	-48.749	1.00	28.65	RNA2	N
ATOM	3360	C4	U	D1078	6.455	-16.177	-48.357	1.00	30.34	RNA2	C
ATOM	3361	O4	U	D1078	7.555	-16.119	-47.795	1.00	39.15	RNA2	O
ATOM	3362	C5	U	D1078	5.749	-17.376	-48.699	1.00	25.89	RNA2	C
ATOM	3363	C6	U	D1078	4.584	-17.300	-49.355	1.00	28.67	RNA2	C
ATOM	3364	P	C	D1079	2.674	-18.503	-54.775	1.00	37.89	RNA2	P
ATOM	3365	O1P	C	D1079	2.944	-18.013	-56.153	1.00	39.80	RNA2	O
ATOM	3366	O2P	C	D1079	3.558	-19.539	-54.176	1.00	37.02	RNA2	O
ATOM	3367	O5*	C	D1079	1.167	-18.996	-54.704	1.00	15.08	RNA2	O

ATOM 3368 C5* C D1079 0.145 -18.192 -55.288 1.00 23.37 RNA2 C
ATOM 3369 C4* C D1079 -1.208 -18.608 -54.795 1.00 19.59 RNA2 C
ATOM 3370 O4* C D1079 -1.438 -18.079 -53.467 1.00 27.26 RNA2 O
ATOM 3371 C3* C D1079 -2.308 -17.995 -55.628 1.00 31.62 RNA2 C
ATOM 3372 O3* C D1079 -2.525 -18.767 -56.789 1.00 35.58 RNA2 O
ATOM 3373 C2* C D1079 -3.484 -17.941 -54.667 1.00 27.16 RNA2 C
ATOM 3374 O2* C D1079 -4.148 -19.180 -54.551 1.00 30.55 RNA2 O
ATOM 3375 C1* C D1079 -2.774 -17.609 -53.357 1.00 19.20 RNA2 C
ATOM 3376 N1 C D1079 -2.738 -16.155 -53.087 1.00 15.42 RNA2 N
ATOM 3377 C2 C D1079 -3.891 -15.525 -52.594 1.00 14.73 RNA2 C
ATOM 3378 O2 C D1079 -4.922 -16.196 -52.423 1.00 22.43 RNA2 O
ATOM 3379 N3 C D1079 -3.853 -14.203 -52.319 1.00 15.70 RNA2 N
ATOM 3380 C4 C D1079 -2.730 -13.512 -52.513 1.00 19.14 RNA2 C
ATOM 3381 N4 C D1079 -2.733 -12.219 -52.194 1.00 18.52 RNA2 N
ATOM 3382 C5 C D1079 -1.550 -14.119 -53.033 1.00 14.27 RNA2 C
ATOM 3383 C6 C D1079 -1.598 -15.430 -53.303 1.00 9.72 RNA2 C
ATOM 3384 P A D1080 -2.665 -18.025 -58.200 1.00 33.84 RNA2 P
ATOM 3385 O1P A D1080 -1.604 -16.982 -58.302 1.00 29.98 RNA2 O
ATOM 3386 O2P A D1080 -2.762 -19.085 -59.240 1.00 51.18 RNA2 O
ATOM 3387 O5* A D1080 -4.078 -17.315 -58.069 1.00 18.89 RNA2 O
ATOM 3388 C5* A D1080 -5.228 -18.109 -57.802 1.00 23.14 RNA2 C
ATOM 3389 C4* A D1080 -6.362 -17.256 -57.316 1.00 29.15 RNA2 C
ATOM 3390 O4* A D1080 -6.077 -16.724 -55.997 1.00 31.88 RNA2 O
ATOM 3391 C3* A D1080 -6.704 -16.028 -58.131 1.00 27.12 RNA2 C
ATOM 3392 O3* A D1080 -7.427 -16.344 -59.312 1.00 35.45 RNA2 O
ATOM 3393 C2* A D1080 -7.520 -15.221 -57.129 1.00 24.68 RNA2 C
ATOM 3394 O2* A D1080 -8.839 -15.710 -57.002 1.00 23.19 RNA2 O
ATOM 3395 C1* A D1080 -6.774 -15.502 -55.826 1.00 22.08 RNA2 C
ATOM 3396 N9 A D1080 -5.817 -14.431 -55.545 1.00 19.19 RNA2 N
ATOM 3397 C8 A D1080 -4.460 -14.391 -55.773 1.00 21.24 RNA2 C
ATOM 3398 N7 A D1080 -3.911 -13.232 -55.485 1.00 17.04 RNA2 N
ATOM 3399 C5 A D1080 -4.974 -12.465 -55.021 1.00 10.07 RNA2 C
ATOM 3400 C6 A D1080 -5.061 -11.132 -54.578 1.00 15.82 RNA2 C
ATOM 3401 N6 A D1080 -4.019 -10.295 -54.529 1.00 19.09 RNA2 N
ATOM 3402 N1 A D1080 -6.271 -10.680 -54.183 1.00 20.36 RNA2 N
ATOM 3403 C2 A D1080 -7.317 -11.517 -54.229 1.00 15.92 RNA2 C
ATOM 3404 N3 A D1080 -7.362 -12.783 -54.626 1.00 14.17 RNA2 N
ATOM 3405 C4 A D1080 -6.145 -13.200 -55.023 1.00 9.63 RNA2 C
ATOM 3406 P U D1081 -7.413 -15.312 -60.548 1.00 31.28 RNA2 P
ATOM 3407 O1P U D1081 -6.027 -14.791 -60.717 1.00 8.76 RNA2 O
ATOM 3408 O2P U D1081 -8.089 -15.971 -61.696 1.00 35.73 RNA2 O
ATOM 3409 O5* U D1081 -8.356 -14.144 -60.021 1.00 18.56 RNA2 O
ATOM 3410 C5* U D1081 -9.643 -14.457 -59.459 1.00 22.44 RNA2 C
ATOM 3411 C4* U D1081 -10.276 -13.222 -58.867 1.00 34.63 RNA2 C
ATOM 3412 O4* U D1081 -9.471 -12.728 -57.771 1.00 31.00 RNA2 O

ATOM 3413 C3* U D1081 -10.406 -12.045 -59.817 1.00 37.02 RNA2 C
ATOM 3414 O3* U D1081 -11.605 -12.172 -60.569 1.00 43.64 RNA2 O
ATOM 3415 C2* U D1081 -10.429 -10.844 -58.874 1.00 32.75 RNA2 C
ATOM 3416 O2* U D1081 -11.714 -10.603 -58.330 1.00 30.48 RNA2 O
ATOM 3417 C1* U D1081 -9.499 -11.311 -57.756 1.00 21.25 RNA2 C
ATOM 3418 N1 U D1081 -8.115 -10.826 -57.857 1.00 8.85 RNA2 N
ATOM 3419 C2 U D1081 -7.839 -9.537 -57.429 1.00 18.01 RNA2 C
ATOM 3420 O2 U D1081 -8.706 -8.754 -57.039 1.00 20.38 RNA2 O
ATOM 3421 N3 U D1081 -6.515 -9.190 -57.477 1.00 4.56 RNA2 N
ATOM 3422 C4 U D1081 -5.463 -9.977 -57.902 1.00 19.29 RNA2 C
ATOM 3423 O4 U D1081 -4.306 -9.560 -57.785 1.00 17.28 RNA2 O
ATOM 3424 C5 U D1081 -5.838 -11.273 -58.364 1.00 8.37 RNA2 C
ATOM 3425 C6 U D1081 -7.118 -11.640 -58.331 1.00 9.01 RNA2 C
ATOM 3426 P U D1082 -11.700 -11.511 -62.026 1.00 37.21 RNA2 P
ATOM 3427 O1P U D1082 -10.555 -11.984 -62.849 1.00 30.04 RNA2 O
ATOM 3428 O2P U D1082 -13.101 -11.726 -62.489 1.00 36.07 RNA2 O
ATOM 3429 O5* U D1082 -11.463 -9.962 -61.755 1.00 48.61 RNA2 O
ATOM 3430 C5* U D1082 -12.470 -9.172 -61.107 1.00 49.13 RNA2 C
ATOM 3431 C4* U D1082 -12.043 -7.729 -61.052 1.00 45.78 RNA2 C
ATOM 3432 O4* U D1082 -11.006 -7.553 -60.054 1.00 41.16 RNA2 O
ATOM 3433 C3* U D1082 -11.417 -7.176 -62.317 1.00 45.00 RNA2 C
ATOM 3434 O3* U D1082 -12.349 -6.822 -63.321 1.00 44.91 RNA2 O
ATOM 3435 C2* U D1082 -10.633 -5.979 -61.801 1.00 41.47 RNA2 C
ATOM 3436 O2* U D1082 -11.449 -4.837 -61.628 1.00 38.13 RNA2 O
ATOM 3437 C1* U D1082 -10.147 -6.497 -60.448 1.00 34.17 RNA2 C
ATOM 3438 N1 U D1082 -8.767 -6.998 -60.524 1.00 21.76 RNA2 N
ATOM 3439 C2 U D1082 -7.752 -6.093 -60.271 1.00 27.58 RNA2 C
ATOM 3440 O2 U D1082 -7.961 -4.925 -59.983 1.00 39.33 RNA2 O
ATOM 3441 N3 U D1082 -6.482 -6.599 -60.370 1.00 17.32 RNA2 N
ATOM 3442 C4 U D1082 -6.125 -7.886 -60.687 1.00 19.81 RNA2 C
ATOM 3443 O4 U D1082 -4.925 -8.184 -60.736 1.00 21.01 RNA2 O
ATOM 3444 C5 U D1082 -7.228 -8.767 -60.933 1.00 16.38 RNA2 C
ATOM 3445 C6 U D1082 -8.483 -8.304 -60.843 1.00 16.69 RNA2 C
ATOM 3446 P U D1083 -11.820 -6.597 -64.817 1.00 43.63 RNA2 P
ATOM 3447 O1P U D1083 -11.131 -7.845 -65.255 1.00 40.26 RNA2 O
ATOM 3448 O2P U D1083 -12.950 -6.055 -65.619 1.00 45.21 RNA2 O
ATOM 3449 O5* U D1083 -10.714 -5.466 -64.618 1.00 33.40 RNA2 O
ATOM 3450 C5* U D1083 -9.461 -5.509 -65.306 1.00 21.92 RNA2 C
ATOM 3451 C4* U D1083 -8.508 -4.519 -64.689 1.00 33.84 RNA2 C
ATOM 3452 O4* U D1083 -7.824 -5.125 -63.563 1.00 30.68 RNA2 O
ATOM 3453 C3* U D1083 -7.392 -4.060 -65.607 1.00 39.61 RNA2 C
ATOM 3454 O3* U D1083 -7.851 -2.983 -66.405 1.00 47.78 RNA2 O
ATOM 3455 C2* U D1083 -6.301 -3.633 -64.635 1.00 38.07 RNA2 C
ATOM 3456 O2* U D1083 -6.517 -2.326 -64.141 1.00 48.19 RNA2 O
ATOM 3457 C1* U D1083 -6.486 -4.647 -63.504 1.00 32.72 RNA2 C

ATOM	3458	N1	U	D1083	-5.568	-5.793	-63.608	1.00	23.49	RNA2	N
ATOM	3459	C2	U	D1083	-4.251	-5.604	-63.225	1.00	27.40	RNA2	C
ATOM	3460	O2	U	D1083	-3.823	-4.541	-62.823	1.00	42.53	RNA2	O
ATOM	3461	N3	U	D1083	-3.447	-6.710	-63.335	1.00	31.74	RNA2	N
ATOM	3462	C4	U	D1083	-3.809	-7.963	-63.784	1.00	30.45	RNA2	C
ATOM	3463	O4	U	D1083	-2.962	-8.863	-63.823	1.00	30.78	RNA2	O
ATOM	3464	C5	U	D1083	-5.183	-8.081	-64.168	1.00	19.97	RNA2	C
ATOM	3465	C6	U	D1083	-5.995	-7.019	-64.069	1.00	27.83	RNA2	C
ATOM	3466	P	A	D1084	-7.438	-2.912	-67.949	1.00	45.35	RNA2	P
ATOM	3467	O1P	A	D1084	-7.390	-4.295	-68.485	1.00	47.07	RNA2	O
ATOM	3468	O2P	A	D1084	-8.323	-1.906	-68.587	1.00	48.86	RNA2	O
ATOM	3469	O5*	A	D1084	-5.952	-2.353	-67.903	1.00	30.12	RNA2	O
ATOM	3470	C5*	A	D1084	-5.051	-2.560	-68.990	1.00	25.41	RNA2	C
ATOM	3471	C4*	A	D1084	-3.717	-1.960	-68.652	1.00	29.72	RNA2	C
ATOM	3472	O4*	A	D1084	-3.876	-0.534	-68.496	1.00	39.52	RNA2	O
ATOM	3473	C3*	A	D1084	-3.174	-2.444	-67.326	1.00	26.49	RNA2	C
ATOM	3474	O3*	A	D1084	-2.405	-3.601	-67.544	1.00	36.34	RNA2	O
ATOM	3475	C2*	A	D1084	-2.346	-1.271	-66.828	1.00	33.86	RNA2	C
ATOM	3476	O2*	A	D1084	-1.043	-1.267	-67.373	1.00	28.54	RNA2	O
ATOM	3477	C1*	A	D1084	-3.138	-0.086	-67.379	1.00	30.15	RNA2	C
ATOM	3478	N9	A	D1084	-4.093	0.522	-66.459	1.00	28.36	RNA2	N
ATOM	3479	C8	A	D1084	-5.439	0.258	-66.342	1.00	28.20	RNA2	C
ATOM	3480	N7	A	D1084	-6.058	1.041	-65.494	1.00	25.56	RNA2	N
ATOM	3481	C5	A	D1084	-5.050	1.861	-65.004	1.00	22.38	RNA2	C
ATOM	3482	C6	A	D1084	-5.061	2.922	-64.088	1.00	27.67	RNA2	C
ATOM	3483	N6	A	D1084	-6.165	3.359	-63.482	1.00	38.68	RNA2	N
ATOM	3484	N1	A	D1084	-3.884	3.530	-63.815	1.00	34.84	RNA2	N
ATOM	3485	C2	A	D1084	-2.776	3.091	-64.434	1.00	37.58	RNA2	C
ATOM	3486	N3	A	D1084	-2.641	2.106	-65.322	1.00	27.16	RNA2	N
ATOM	3487	C4	A	D1084	-3.830	1.530	-65.569	1.00	29.13	RNA2	C
ATOM	3488	P	A	D1085	-2.533	-4.824	-66.531	1.00	33.05	RNA2	P
ATOM	3489	O1P	A	D1085	-3.976	-4.945	-66.187	1.00	26.54	RNA2	O
ATOM	3490	O2P	A	D1085	-1.809	-5.987	-67.103	1.00	37.42	RNA2	O
ATOM	3491	O5*	A	D1085	-1.708	-4.311	-65.275	1.00	37.64	RNA2	O
ATOM	3492	C5*	A	D1085	-0.321	-3.983	-65.415	1.00	34.30	RNA2	C
ATOM	3493	C4*	A	D1085	0.137	-3.193	-64.225	1.00	40.98	RNA2	C
ATOM	3494	O4*	A	D1085	-0.509	-1.900	-64.217	1.00	45.08	RNA2	O
ATOM	3495	C3*	A	D1085	-0.209	-3.817	-62.888	1.00	33.48	RNA2	C
ATOM	3496	O3*	A	D1085	0.816	-4.734	-62.538	1.00	33.50	RNA2	O
ATOM	3497	C2*	A	D1085	-0.260	-2.614	-61.955	1.00	33.78	RNA2	C
ATOM	3498	O2*	A	D1085	1.022	-2.252	-61.488	1.00	36.97	RNA2	O
ATOM	3499	C1*	A	D1085	-0.762	-1.506	-62.885	1.00	29.69	RNA2	C
ATOM	3500	N9	A	D1085	-2.183	-1.205	-62.769	1.00	20.61	RNA2	N
ATOM	3501	C8	A	D1085	-3.232	-1.910	-63.299	1.00	32.48	RNA2	C
ATOM	3502	N7	A	D1085	-4.406	-1.388	-63.038	1.00	31.65	RNA2	N

ATOM 3503 C5 A D1085 -4.110 -0.263 -62.285 1.00 23.98 RNA2 C
ATOM 3504 C6 A D1085 -4.922 0.724 -61.710 1.00 27.87 RNA2 C
ATOM 3505 N6 A D1085 -6.253 0.732 -61.813 1.00 35.25 RNA2 N
ATOM 3506 N1 A D1085 -4.315 1.716 -61.023 1.00 23.17 RNA2 N
ATOM 3507 C2 A D1085 -2.975 1.709 -60.936 1.00 28.66 RNA2 C
ATOM 3508 N3 A D1085 -2.102 0.838 -61.439 1.00 29.00 RNA2 N
ATOM 3509 C4 A D1085 -2.742 -0.137 -62.110 1.00 24.43 RNA2 C
ATOM 3510 P A D1086 0.438 -6.094 -61.782 1.00 32.76 RNA2 P
ATOM 3511 O1P A D1086 -0.961 -6.454 -62.137 1.00 17.94 RNA2 O
ATOM 3512 O2P A D1086 1.532 -7.068 -62.001 1.00 30.14 RNA2 O
ATOM 3513 O5* A D1086 0.451 -5.671 -60.253 1.00 42.21 RNA2 O
ATOM 3514 C5* A D1086 1.644 -5.155 -59.645 1.00 32.88 RNA2 C
ATOM 3515 C4* A D1086 1.288 -4.326 -58.440 1.00 36.41 RNA2 C
ATOM 3516 O4* A D1086 0.612 -3.114 -58.860 1.00 29.39 RNA2 O
ATOM 3517 C3* A D1086 0.303 -4.967 -57.481 1.00 36.90 RNA2 C
ATOM 3518 O3* A D1086 0.922 -5.900 -56.613 1.00 33.24 RNA2 O
ATOM 3519 C2* A D1086 -0.287 -3.768 -56.748 1.00 42.63 RNA2 C
ATOM 3520 O2* A D1086 0.470 -3.347 -55.630 1.00 53.18 RNA2 O
ATOM 3521 C1* A D1086 -0.267 -2.692 -57.839 1.00 38.42 RNA2 C
ATOM 3522 N9 A D1086 -1.590 -2.432 -58.407 1.00 27.17 RNA2 N
ATOM 3523 C8 A D1086 -2.195 -1.210 -58.569 1.00 27.28 RNA2 C
ATOM 3524 N7 A D1086 -3.431 -1.285 -59.001 1.00 32.05 RNA2 N
ATOM 3525 C5 A D1086 -3.644 -2.647 -59.160 1.00 25.72 RNA2 C
ATOM 3526 C6 A D1086 -4.765 -3.385 -59.572 1.00 30.69 RNA2 C
ATOM 3527 N6 A D1086 -5.930 -2.832 -59.910 1.00 37.15 RNA2 N
ATOM 3528 N1 A D1086 -4.650 -4.731 -59.619 1.00 26.67 RNA2 N
ATOM 3529 C2 A D1086 -3.484 -5.284 -59.271 1.00 27.74 RNA2 C
ATOM 3530 N3 A D1086 -2.360 -4.697 -58.860 1.00 32.46 RNA2 N
ATOM 3531 C4 A D1086 -2.510 -3.363 -58.824 1.00 28.26 RNA2 C
ATOM 3532 P G D1087 0.286 -7.364 -56.455 1.00 31.77 RNA2 P
ATOM 3533 O1P G D1087 -0.973 -7.249 -55.682 1.00 28.82 RNA2 O
ATOM 3534 O2P G D1087 0.266 -8.020 -57.788 1.00 46.35 RNA2 O
ATOM 3535 O5* G D1087 1.337 -8.122 -55.545 1.00 32.87 RNA2 O
ATOM 3536 C5* G D1087 2.401 -8.899 -56.109 1.00 29.23 RNA2 C
ATOM 3537 C4* G D1087 3.449 -9.109 -55.061 1.00 33.39 RNA2 C
ATOM 3538 O4* G D1087 4.062 -7.829 -54.802 1.00 39.61 RNA2 O
ATOM 3539 C3* G D1087 2.847 -9.568 -53.742 1.00 26.85 RNA2 C
ATOM 3540 O3* G D1087 2.937 -10.985 -53.689 1.00 26.33 RNA2 O
ATOM 3541 C2* G D1087 3.745 -8.914 -52.696 1.00 29.63 RNA2 C
ATOM 3542 O2* G D1087 4.887 -9.702 -52.418 1.00 30.88 RNA2 O
ATOM 3543 C1* G D1087 4.196 -7.635 -53.412 1.00 31.58 RNA2 C
ATOM 3544 N9 G D1087 3.534 -6.370 -53.099 1.00 24.38 RNA2 N
ATOM 3545 C8 G D1087 2.184 -6.105 -53.015 1.00 13.22 RNA2 C
ATOM 3546 N7 G D1087 1.926 -4.837 -52.821 1.00 6.56 RNA2 N
ATOM 3547 C5 G D1087 3.176 -4.240 -52.743 1.00 11.78 RNA2 C

ATOM	3548	C6	G	D1087	3.536	-2.887	-52.546	1.00	26.38	RNA2	C
ATOM	3549	O6	G	D1087	2.796	-1.905	-52.394	1.00	28.30	RNA2	O
ATOM	3550	N1	G	D1087	4.919	-2.723	-52.537	1.00	19.38	RNA2	N
ATOM	3551	C2	G	D1087	5.836	-3.736	-52.697	1.00	26.46	RNA2	C
ATOM	3552	N2	G	D1087	7.138	-3.390	-52.661	1.00	19.48	RNA2	N
ATOM	3553	N3	G	D1087	5.509	-4.997	-52.881	1.00	20.61	RNA2	N
ATOM	3554	C4	G	D1087	4.176	-5.176	-52.894	1.00	16.45	RNA2	C
ATOM	3555	P	A	D1088	1.639	-11.888	-53.962	1.00	30.91	RNA2	P
ATOM	3556	O1P	A	D1088	0.713	-11.203	-54.900	1.00	35.03	RNA2	O
ATOM	3557	O2P	A	D1088	2.152	-13.234	-54.286	1.00	39.93	RNA2	O
ATOM	3558	O5*	A	D1088	0.937	-11.965	-52.543	1.00	35.70	RNA2	O
ATOM	3559	C5*	A	D1088	1.728	-12.195	-51.367	1.00	40.71	RNA2	C
ATOM	3560	C4*	A	D1088	1.473	-11.114	-50.352	1.00	31.86	RNA2	C
ATOM	3561	O4*	A	D1088	0.051	-11.035	-50.098	1.00	31.43	RNA2	O
ATOM	3562	C3*	A	D1088	2.134	-11.354	-49.008	1.00	28.62	RNA2	C
ATOM	3563	O3*	A	D1088	2.454	-10.092	-48.453	1.00	22.01	RNA2	O
ATOM	3564	C2*	A	D1088	1.032	-12.007	-48.192	1.00	19.87	RNA2	C
ATOM	3565	O2*	A	D1088	1.196	-11.783	-46.811	1.00	35.87	RNA2	O
ATOM	3566	C1*	A	D1088	-0.209	-11.301	-48.739	1.00	17.80	RNA2	C
ATOM	3567	N9	A	D1088	-1.421	-12.106	-48.687	1.00	8.11	RNA2	N
ATOM	3568	C8	A	D1088	-2.654	-11.733	-48.221	1.00	11.14	RNA2	C
ATOM	3569	N7	A	D1088	-3.559	-12.675	-48.317	1.00	26.75	RNA2	N
ATOM	3570	C5	A	D1088	-2.873	-13.743	-48.883	1.00	15.31	RNA2	C
ATOM	3571	C6	A	D1088	-3.272	-15.045	-49.241	1.00	15.70	RNA2	C
ATOM	3572	N6	A	D1088	-4.511	-15.516	-49.067	1.00	17.72	RNA2	N
ATOM	3573	N1	A	D1088	-2.343	-15.856	-49.789	1.00	9.16	RNA2	N
ATOM	3574	C2	A	D1088	-1.099	-15.388	-49.957	1.00	14.79	RNA2	C
ATOM	3575	N3	A	D1088	-0.603	-14.189	-49.657	1.00	18.20	RNA2	N
ATOM	3576	C4	A	D1088	-1.555	-13.405	-49.117	1.00	14.12	RNA2	C
ATOM	3577	P	G	D1089	3.501	-9.994	-47.248	1.00	27.70	RNA2	P
ATOM	3578	O1P	G	D1089	4.147	-11.322	-47.068	1.00	28.27	RNA2	O
ATOM	3579	O2P	G	D1089	2.776	-9.361	-46.117	1.00	25.52	RNA2	O
ATOM	3580	O5*	G	D1089	4.606	-8.988	-47.785	1.00	22.53	RNA2	O
ATOM	3581	C5*	G	D1089	5.471	-9.357	-48.871	1.00	30.86	RNA2	C
ATOM	3582	C4*	G	D1089	5.959	-8.118	-49.573	1.00	24.73	RNA2	C
ATOM	3583	O4*	G	D1089	4.810	-7.428	-50.122	1.00	31.53	RNA2	O
ATOM	3584	C3*	G	D1089	6.676	-7.119	-48.676	1.00	23.96	RNA2	C
ATOM	3585	O3*	G	D1089	7.692	-6.491	-49.437	1.00	35.59	RNA2	O
ATOM	3586	C2*	G	D1089	5.581	-6.109	-48.333	1.00	26.26	RNA2	C
ATOM	3587	O2*	G	D1089	6.055	-4.799	-48.099	1.00	39.73	RNA2	O
ATOM	3588	C1*	G	D1089	4.742	-6.120	-49.602	1.00	26.61	RNA2	C
ATOM	3589	N9	G	D1089	3.339	-5.773	-49.400	1.00	22.30	RNA2	N
ATOM	3590	C8	G	D1089	2.265	-6.629	-49.311	1.00	19.61	RNA2	C
ATOM	3591	N7	G	D1089	1.123	-6.007	-49.184	1.00	20.16	RNA2	N
ATOM	3592	C5	G	D1089	1.468	-4.661	-49.171	1.00	20.55	RNA2	C

ATOM	3593	C6	G	D1089	0.653	-3.505	-49.059	1.00	26.65	RNA2 C
ATOM	3594	O6	G	D1089	-0.582	-3.435	-48.934	1.00	34.44	RNA2 O
ATOM	3595	N1	G	D1089	1.415	-2.339	-49.098	1.00	18.23	RNA2 N
ATOM	3596	C2	G	D1089	2.782	-2.292	-49.218	1.00	22.47	RNA2 C
ATOM	3597	N2	G	D1089	3.341	-1.065	-49.215	1.00	23.99	RNA2 N
ATOM	3598	N3	G	D1089	3.551	-3.365	-49.325	1.00	21.65	RNA2 N
ATOM	3599	C4	G	D1089	2.832	-4.504	-49.293	1.00	15.76	RNA2 C
ATOM	3600	P	U	D1090	9.177	-7.107	-49.459	1.00	46.88	RNA2 P
ATOM	3601	O1P	U	D1090	9.375	-7.944	-48.246	1.00	47.63	RNA2 O
ATOM	3602	O2P	U	D1090	9.376	-7.711	-50.800	1.00	46.50	RNA2 O
ATOM	3603	O5*	U	D1090	10.098	-5.811	-49.333	1.00	47.06	RNA2 O
ATOM	3604	C5*	U	D1090	11.428	-5.782	-49.876	1.00	48.58	RNA2 C
ATOM	3605	C4*	U	D1090	12.040	-4.407	-49.703	1.00	55.86	RNA2 C
ATOM	3606	O4*	U	D1090	11.307	-3.422	-50.482	1.00	58.42	RNA2 O
ATOM	3607	C3*	U	D1090	12.027	-3.835	-48.296	1.00	57.85	RNA2 C
ATOM	3608	O3*	U	D1090	13.074	-4.330	-47.488	1.00	54.72	RNA2 O
ATOM	3609	C2*	U	D1090	12.152	-2.336	-48.538	1.00	56.90	RNA2 C
ATOM	3610	O2*	U	D1090	13.486	-1.912	-48.750	1.00	55.53	RNA2 O
ATOM	3611	C1*	U	D1090	11.345	-2.164	-49.823	1.00	47.41	RNA2 C
ATOM	3612	N1	U	D1090	9.971	-1.713	-49.552	1.00	39.04	RNA2 N
ATOM	3613	C2	U	D1090	9.769	-0.350	-49.369	1.00	41.49	RNA2 C
ATOM	3614	O2	U	D1090	10.675	0.475	-49.415	1.00	47.92	RNA2 O
ATOM	3615	N3	U	D1090	8.468	0.014	-49.123	1.00	33.29	RNA2 N
ATOM	3616	C4	U	D1090	7.371	-0.820	-49.033	1.00	35.37	RNA2 C
ATOM	3617	O4	U	D1090	6.255	-0.333	-48.820	1.00	43.33	RNA2 O
ATOM	3618	C5	U	D1090	7.660	-2.210	-49.227	1.00	26.33	RNA2 C
ATOM	3619	C6	U	D1090	8.916	-2.599	-49.476	1.00	31.79	RNA2 C
ATOM	3620	P	G	D1091	12.865	-4.400	-45.899	1.00	63.03	RNA2 P
ATOM	3621	O1P	G	D1091	11.489	-4.915	-45.629	1.00	48.47	RNA2 O
ATOM	3622	O2P	G	D1091	14.047	-5.119	-45.346	1.00	63.48	RNA2 O
ATOM	3623	O5*	G	D1091	12.909	-2.874	-45.434	1.00	53.82	RNA2 O
ATOM	3624	C5*	G	D1091	14.160	-2.173	-45.369	1.00	60.37	RNA2 C
ATOM	3625	C4*	G	D1091	13.939	-0.687	-45.231	1.00	57.35	RNA2 C
ATOM	3626	O4*	G	D1091	13.057	-0.232	-46.291	1.00	51.52	RNA2 O
ATOM	3627	C3*	G	D1091	13.275	-0.168	-43.964	1.00	64.14	RNA2 C
ATOM	3628	O3*	G	D1091	14.165	-0.050	-42.851	1.00	71.95	RNA2 O
ATOM	3629	C2*	G	D1091	12.766	1.197	-44.414	1.00	59.80	RNA2 C
ATOM	3630	O2*	G	D1091	13.774	2.190	-44.402	1.00	67.83	RNA2 O
ATOM	3631	C1*	G	D1091	12.345	0.913	-45.854	1.00	48.17	RNA2 C
ATOM	3632	N9	G	D1091	10.912	0.647	-45.911	1.00	35.24	RNA2 N
ATOM	3633	C8	G	D1091	10.281	-0.571	-45.991	1.00	35.20	RNA2 C
ATOM	3634	N7	G	D1091	8.979	-0.474	-45.954	1.00	29.59	RNA2 N
ATOM	3635	C5	G	D1091	8.739	0.890	-45.858	1.00	21.43	RNA2 C
ATOM	3636	C6	G	D1091	7.518	1.604	-45.771	1.00	32.33	RNA2 C
ATOM	3637	O6	G	D1091	6.364	1.159	-45.749	1.00	43.19	RNA2 O

ATOM	3638	N1	G	D1091	7.731	2.976	-45.699	1.00	28.62	RNA2 N
ATOM	3639	C2	G	D1091	8.961	3.582	-45.701	1.00	39.37	RNA2 C
ATOM	3640	N2	G	D1091	8.965	4.920	-45.626	1.00	34.96	RNA2 N
ATOM	3641	N3	G	D1091	10.107	2.925	-45.772	1.00	32.50	RNA2 N
ATOM	3642	C4	G	D1091	9.920	1.594	-45.848	1.00	25.53	RNA2 C
ATOM	3643	P	C	D1092	13.560	0.093	-41.358	1.00	80.57	RNA2 P
ATOM	3644	O1P	C	D1092	12.499	-0.941	-41.171	1.00	72.16	RNA2 O
ATOM	3645	O2P	C	D1092	14.702	0.146	-40.409	1.00	77.36	RNA2 O
ATOM	3646	O5*	C	D1092	12.841	1.520	-41.356	1.00	67.00	RNA2 O
ATOM	3647	C5*	C	D1092	13.608	2.728	-41.517	1.00	47.50	RNA2 C
ATOM	3648	C4*	C	D1092	12.721	3.950	-41.413	1.00	46.89	RNA2 C
ATOM	3649	O4*	C	D1092	11.785	3.999	-42.524	1.00	47.64	RNA2 O
ATOM	3650	C3*	C	D1092	11.825	4.069	-40.193	1.00	48.58	RNA2 C
ATOM	3651	O3*	C	D1092	12.485	4.523	-39.029	1.00	50.53	RNA2 O
ATOM	3652	C2*	C	D1092	10.775	5.069	-40.650	1.00	46.94	RNA2 C
ATOM	3653	O2*	C	D1092	11.196	6.411	-40.524	1.00	56.76	RNA2 O
ATOM	3654	C1*	C	D1092	10.610	4.694	-42.122	1.00	44.37	RNA2 C
ATOM	3655	N1	C	D1092	9.429	3.823	-42.282	1.00	40.91	RNA2 N
ATOM	3656	C2	C	D1092	8.155	4.415	-42.217	1.00	43.01	RNA2 C
ATOM	3657	O2	C	D1092	8.072	5.647	-42.083	1.00	41.14	RNA2 O
ATOM	3658	N3	C	D1092	7.056	3.632	-42.298	1.00	33.92	RNA2 N
ATOM	3659	C4	C	D1092	7.188	2.312	-42.444	1.00	39.14	RNA2 C
ATOM	3660	N4	C	D1092	6.075	1.577	-42.496	1.00	35.85	RNA2 N
ATOM	3661	C5	C	D1092	8.469	1.685	-42.538	1.00	31.59	RNA2 C
ATOM	3662	C6	C	D1092	9.552	2.471	-42.458	1.00	35.03	RNA2 C
ATOM	3663	P	G	D1093	11.977	4.012	-37.593	1.00	51.96	RNA2 P
ATOM	3664	O1P	G	D1093	11.975	2.526	-37.626	1.00	48.41	RNA2 O
ATOM	3665	O2P	G	D1093	12.764	4.724	-36.553	1.00	64.77	RNA2 O
ATOM	3666	O5*	G	D1093	10.458	4.492	-37.515	1.00	35.20	RNA2 O
ATOM	3667	C5*	G	D1093	10.122	5.886	-37.581	1.00	24.69	RNA2 C
ATOM	3668	C4*	G	D1093	8.630	6.056	-37.704	1.00	29.37	RNA2 C
ATOM	3669	O4*	G	D1093	8.164	5.435	-38.930	1.00	34.30	RNA2 O
ATOM	3670	C3*	G	D1093	7.808	5.387	-36.620	1.00	33.91	RNA2 C
ATOM	3671	O3*	G	D1093	7.738	6.175	-35.452	1.00	53.14	RNA2 O
ATOM	3672	C2*	G	D1093	6.454	5.194	-37.289	1.00	36.57	RNA2 C
ATOM	3673	O2*	G	D1093	5.628	6.344	-37.254	1.00	23.38	RNA2 O
ATOM	3674	C1*	G	D1093	6.871	4.878	-38.726	1.00	33.38	RNA2 C
ATOM	3675	N9	G	D1093	6.940	3.436	-38.961	1.00	31.32	RNA2 N
ATOM	3676	C8	G	D1093	8.073	2.656	-39.054	1.00	27.97	RNA2 C
ATOM	3677	N7	G	D1093	7.812	1.389	-39.243	1.00	30.70	RNA2 N
ATOM	3678	C5	G	D1093	6.424	1.326	-39.280	1.00	27.66	RNA2 C
ATOM	3679	C6	G	D1093	5.563	0.215	-39.451	1.00	30.04	RNA2 C
ATOM	3680	O6	G	D1093	5.866	-0.977	-39.608	1.00	42.76	RNA2 O
ATOM	3681	N1	G	D1093	4.222	0.596	-39.422	1.00	21.84	RNA2 N
ATOM	3682	C2	G	D1093	3.770	1.881	-39.247	1.00	13.29	RNA2 C

ATOM	3683	N2	G	D1093	2.437	2.046	-39.237	1.00	19.33	RNA2	N
ATOM	3684	N3	G	D1093	4.564	2.926	-39.091	1.00	16.91	RNA2	N
ATOM	3685	C4	G	D1093	5.869	2.579	-39.115	1.00	23.30	RNA2	C
ATOM	3686	P	U	D1094	7.627	5.455	-34.022	1.00	46.64	RNA2	P
ATOM	3687	O1P	U	D1094	8.556	4.303	-34.026	1.00	32.38	RNA2	O
ATOM	3688	O2P	U	D1094	7.774	6.516	-32.989	1.00	56.93	RNA2	O
ATOM	3689	O5*	U	D1094	6.124	4.934	-33.989	1.00	26.86	RNA2	O
ATOM	3690	C5*	U	D1094	5.051	5.877	-33.932	1.00	35.20	RNA2	C
ATOM	3691	C4*	U	D1094	3.735	5.172	-33.742	1.00	45.98	RNA2	C
ATOM	3692	O4*	U	D1094	3.308	4.545	-34.978	1.00	50.88	RNA2	O
ATOM	3693	C3*	U	D1094	3.692	4.055	-32.717	1.00	39.85	RNA2	C
ATOM	3694	O3*	U	D1094	3.600	4.551	-31.387	1.00	48.03	RNA2	O
ATOM	3695	C2*	U	D1094	2.457	3.270	-33.154	1.00	40.06	RNA2	C
ATOM	3696	O2*	U	D1094	1.243	3.843	-32.701	1.00	44.52	RNA2	O
ATOM	3697	C1*	U	D1094	2.527	3.400	-34.678	1.00	45.26	RNA2	C
ATOM	3698	N1	U	D1094	3.134	2.217	-35.313	1.00	38.99	RNA2	N
ATOM	3699	C2	U	D1094	2.294	1.148	-35.606	1.00	29.79	RNA2	C
ATOM	3700	O2	U	D1094	1.083	1.180	-35.422	1.00	31.88	RNA2	O
ATOM	3701	N3	U	D1094	2.920	0.043	-36.124	1.00	17.61	RNA2	N
ATOM	3702	C4	U	D1094	4.262	-0.105	-36.384	1.00	31.42	RNA2	C
ATOM	3703	O4	U	D1094	4.679	-1.193	-36.785	1.00	23.03	RNA2	O
ATOM	3704	C5	U	D1094	5.062	1.053	-36.093	1.00	28.82	RNA2	C
ATOM	3705	C6	U	D1094	4.485	2.147	-35.584	1.00	23.80	RNA2	C
ATOM	3706	P	A	D1095	4.523	3.907	-30.234	1.00	43.63	RNA2	P
ATOM	3707	O1P	A	D1095	5.870	3.607	-30.802	1.00	36.61	RNA2	O
ATOM	3708	O2P	A	D1095	4.416	4.772	-29.033	1.00	64.56	RNA2	O
ATOM	3709	O5*	A	D1095	3.794	2.535	-29.896	1.00	28.91	RNA2	O
ATOM	3710	C5*	A	D1095	4.511	1.451	-29.281	1.00	29.01	RNA2	C
ATOM	3711	C4*	A	D1095	3.579	0.291	-29.049	1.00	27.64	RNA2	C
ATOM	3712	O4*	A	D1095	2.506	0.741	-28.191	1.00	38.10	RNA2	O
ATOM	3713	C3*	A	D1095	2.890	-0.216	-30.302	1.00	32.19	RNA2	C
ATOM	3714	O3*	A	D1095	3.698	-1.186	-30.964	1.00	40.82	RNA2	O
ATOM	3715	C2*	A	D1095	1.575	-0.772	-29.769	1.00	37.08	RNA2	C
ATOM	3716	O2*	A	D1095	1.705	-2.077	-29.240	1.00	37.59	RNA2	O
ATOM	3717	C1*	A	D1095	1.278	0.195	-28.623	1.00	27.61	RNA2	C
ATOM	3718	N9	A	D1095	0.397	1.313	-28.956	1.00	26.65	RNA2	N
ATOM	3719	C8	A	D1095	0.753	2.601	-29.290	1.00	20.45	RNA2	C
ATOM	3720	N7	A	D1095	-0.273	3.404	-29.463	1.00	27.16	RNA2	N
ATOM	3721	C5	A	D1095	-1.376	2.587	-29.246	1.00	16.61	RNA2	C
ATOM	3722	C6	A	D1095	-2.765	2.837	-29.271	1.00	25.70	RNA2	C
ATOM	3723	N6	A	D1095	-3.303	4.034	-29.520	1.00	29.59	RNA2	N
ATOM	3724	N1	A	D1095	-3.596	1.799	-29.023	1.00	28.34	RNA2	N
ATOM	3725	C2	A	D1095	-3.060	0.599	-28.761	1.00	25.38	RNA2	C
ATOM	3726	N3	A	D1095	-1.775	0.240	-28.702	1.00	28.20	RNA2	N
ATOM	3727	C4	A	D1095	-0.977	1.292	-28.955	1.00	21.18	RNA2	C

ATOM	3728	P	A	D1096	3.829	-1.151	-32.569	1.00	34.70	RNA2	P
ATOM	3729	O1P	A	D1096	4.017	0.256	-32.992	1.00	37.33	RNA2	O
ATOM	3730	O2P	A	D1096	4.838	-2.167	-32.962	1.00	24.34	RNA2	O
ATOM	3731	O5*	A	D1096	2.383	-1.617	-33.047	1.00	20.77	RNA2	O
ATOM	3732	C5*	A	D1096	1.913	-2.930	-32.724	1.00	19.81	RNA2	C
ATOM	3733	C4*	A	D1096	0.421	-3.021	-32.910	1.00	22.36	RNA2	C
ATOM	3734	O4*	A	D1096	-0.262	-2.200	-31.934	1.00	23.18	RNA2	O
ATOM	3735	C3*	A	D1096	-0.119	-2.546	-34.243	1.00	23.44	RNA2	C
ATOM	3736	O3*	A	D1096	0.028	-3.536	-35.249	1.00	37.12	RNA2	O
ATOM	3737	C2*	A	D1096	-1.575	-2.237	-33.914	1.00	26.79	RNA2	C
ATOM	3738	O2*	A	D1096	-2.392	-3.387	-33.889	1.00	29.84	RNA2	O
ATOM	3739	C1*	A	D1096	-1.458	-1.686	-32.493	1.00	23.36	RNA2	C
ATOM	3740	N9	A	D1096	-1.373	-0.228	-32.496	1.00	24.90	RNA2	N
ATOM	3741	C8	A	D1096	-0.240	0.551	-32.560	1.00	30.09	RNA2	C
ATOM	3742	N7	A	D1096	-0.485	1.838	-32.573	1.00	29.53	RNA2	N
ATOM	3743	C5	A	D1096	-1.870	1.914	-32.507	1.00	21.47	RNA2	C
ATOM	3744	C6	A	D1096	-2.751	3.005	-32.479	1.00	23.47	RNA2	C
ATOM	3745	N6	A	D1096	-2.348	4.281	-32.511	1.00	30.56	RNA2	N
ATOM	3746	N1	A	D1096	-4.075	2.741	-32.411	1.00	23.77	RNA2	N
ATOM	3747	C2	A	D1096	-4.471	1.460	-32.368	1.00	24.81	RNA2	C
ATOM	3748	N3	A	D1096	-3.736	0.349	-32.383	1.00	22.60	RNA2	N
ATOM	3749	C4	A	D1096	-2.429	0.650	-32.454	1.00	13.49	RNA2	C
ATOM	3750	P	C	D1097	0.158	-3.087	-36.781	1.00	28.43	RNA2	P
ATOM	3751	O1P	C	D1097	1.274	-2.107	-36.889	1.00	25.96	RNA2	O
ATOM	3752	O2P	C	D1097	0.208	-4.341	-37.575	1.00	39.67	RNA2	O
ATOM	3753	O5*	C	D1097	-1.234	-2.357	-37.037	1.00	17.23	RNA2	O
ATOM	3754	C5*	C	D1097	-1.317	-1.078	-37.691	1.00	20.94	RNA2	C
ATOM	3755	C4*	C	D1097	-2.742	-0.584	-37.636	1.00	29.32	RNA2	C
ATOM	3756	O4*	C	D1097	-3.029	-0.045	-36.315	1.00	40.36	RNA2	O
ATOM	3757	C3*	C	D1097	-3.106	0.550	-38.569	1.00	29.37	RNA2	C
ATOM	3758	O3*	C	D1097	-3.388	0.082	-39.870	1.00	44.58	RNA2	O
ATOM	3759	C2*	C	D1097	-4.341	1.126	-37.895	1.00	33.92	RNA2	C
ATOM	3760	O2*	C	D1097	-5.487	0.330	-38.113	1.00	32.32	RNA2	O
ATOM	3761	C1*	C	D1097	-3.945	1.037	-36.423	1.00	34.10	RNA2	C
ATOM	3762	N1	C	D1097	-3.265	2.289	-36.012	1.00	31.44	RNA2	N
ATOM	3763	C2	C	D1097	-4.047	3.417	-35.683	1.00	27.94	RNA2	C
ATOM	3764	O2	C	D1097	-5.285	3.313	-35.669	1.00	29.21	RNA2	O
ATOM	3765	N3	C	D1097	-3.427	4.588	-35.390	1.00	30.98	RNA2	N
ATOM	3766	C4	C	D1097	-2.090	4.658	-35.404	1.00	44.95	RNA2	C
ATOM	3767	N4	C	D1097	-1.519	5.838	-35.133	1.00	50.64	RNA2	N
ATOM	3768	C5	C	D1097	-1.275	3.522	-35.698	1.00	39.09	RNA2	C
ATOM	3769	C6	C	D1097	-1.897	2.370	-35.988	1.00	32.35	RNA2	C
ATOM	3770	P	A	D1098	-2.688	0.785	-41.132	1.00	43.71	RNA2	P
ATOM	3771	O1P	A	D1098	-1.216	0.563	-41.059	1.00	24.08	RNA2	O
ATOM	3772	O2P	A	D1098	-3.449	0.343	-42.334	1.00	56.53	RNA2	O

ATOM	3773	O5*	A	D1098	-2.952	2.337	-40.908	1.00	42.07	RNA2	O
ATOM	3774	C5*	A	D1098	-4.281	2.842	-40.702	1.00	41.90	RNA2	C
ATOM	3775	C4*	A	D1098	-4.225	4.295	-40.292	1.00	49.33	RNA2	C
ATOM	3776	O4*	A	D1098	-3.523	4.414	-39.025	1.00	47.73	RNA2	O
ATOM	3777	C3*	A	D1098	-3.462	5.219	-41.229	1.00	50.90	RNA2	C
ATOM	3778	O3*	A	D1098	-4.263	5.645	-42.324	1.00	54.47	RNA2	O
ATOM	3779	C2*	A	D1098	-3.057	6.363	-40.303	1.00	47.39	RNA2	C
ATOM	3780	O2*	A	D1098	-4.104	7.289	-40.085	1.00	53.57	RNA2	O
ATOM	3781	C1*	A	D1098	-2.781	5.621	-38.995	1.00	36.88	RNA2	C
ATOM	3782	N9	A	D1098	-1.365	5.289	-38.851	1.00	28.68	RNA2	N
ATOM	3783	C8	A	D1098	-0.744	4.078	-39.051	1.00	36.76	RNA2	C
ATOM	3784	N7	A	D1098	0.560	4.120	-38.906	1.00	27.01	RNA2	N
ATOM	3785	C5	A	D1098	0.813	5.442	-38.575	1.00	32.11	RNA2	C
ATOM	3786	C6	A	D1098	2.004	6.136	-38.311	1.00	39.08	RNA2	C
ATOM	3787	N6	A	D1098	3.217	5.578	-38.364	1.00	35.79	RNA2	N
ATOM	3788	N1	A	D1098	1.907	7.447	-37.996	1.00	37.08	RNA2	N
ATOM	3789	C2	A	D1098	0.692	8.013	-37.969	1.00	35.02	RNA2	C
ATOM	3790	N3	A	D1098	-0.498	7.470	-38.214	1.00	31.17	RNA2	N
ATOM	3791	C4	A	D1098	-0.366	6.169	-38.516	1.00	35.12	RNA2	C
ATOM	3792	P	G	D1099	-3.598	5.799	-43.783	1.00	57.31	RNA2	P
ATOM	3793	O1P	G	D1099	-3.062	4.481	-44.215	1.00	60.32	RNA2	O
ATOM	3794	O2P	G	D1099	-4.589	6.508	-44.640	1.00	60.85	RNA2	O
ATOM	3795	O5*	G	D1099	-2.349	6.753	-43.537	1.00	41.11	RNA2	O
ATOM	3796	C5*	G	D1099	-2.543	8.130	-43.169	1.00	50.07	RNA2	C
ATOM	3797	C4*	G	D1099	-1.216	8.782	-42.888	1.00	47.05	RNA2	C
ATOM	3798	O4*	G	D1099	-0.626	8.173	-41.712	1.00	46.92	RNA2	O
ATOM	3799	C3*	G	D1099	-0.174	8.588	-43.975	1.00	54.47	RNA2	C
ATOM	3800	O3*	G	D1099	-0.305	9.517	-45.036	1.00	55.05	RNA2	O
ATOM	3801	C2*	G	D1099	1.139	8.720	-43.217	1.00	48.61	RNA2	C
ATOM	3802	O2*	G	D1099	1.553	10.057	-43.029	1.00	55.32	RNA2	O
ATOM	3803	C1*	G	D1099	0.781	8.073	-41.878	1.00	40.34	RNA2	C
ATOM	3804	N9	G	D1099	1.140	6.659	-41.891	1.00	34.55	RNA2	N
ATOM	3805	C8	G	D1099	0.293	5.577	-41.965	1.00	33.18	RNA2	C
ATOM	3806	N7	G	D1099	0.926	4.437	-42.047	1.00	37.87	RNA2	N
ATOM	3807	C5	G	D1099	2.270	4.787	-42.007	1.00	28.79	RNA2	C
ATOM	3808	C6	G	D1099	3.437	3.978	-42.083	1.00	36.73	RNA2	C
ATOM	3809	O6	G	D1099	3.519	2.747	-42.210	1.00	46.32	RNA2	O
ATOM	3810	N1	G	D1099	4.596	4.744	-42.006	1.00	30.92	RNA2	N
ATOM	3811	C2	G	D1099	4.630	6.113	-41.873	1.00	40.47	RNA2	C
ATOM	3812	N2	G	D1099	5.847	6.678	-41.812	1.00	23.42	RNA2	N
ATOM	3813	N3	G	D1099	3.549	6.876	-41.805	1.00	31.10	RNA2	N
ATOM	3814	C4	G	D1099	2.415	6.152	-41.883	1.00	28.17	RNA2	C
ATOM	3815	P	C	D1100	0.097	9.071	-46.522	1.00	56.56	RNA2	P
ATOM	3816	O1P	C	D1100	-0.323	7.657	-46.716	1.00	63.87	RNA2	O
ATOM	3817	O2P	C	D1100	-0.407	10.115	-47.447	1.00	69.36	RNA2	O

ATOM	3818	O5*	C	D	1100	1.688	9.106	-46.507	1.00 39.12	RNA2 O
ATOM	3819	C5*	C	D	1100	2.380	10.337	-46.298	1.00 32.71	RNA2 C
ATOM	3820	C4*	C	D	1100	3.863	10.098	-46.207	1.00 40.37	RNA2 C
ATOM	3821	O4*	C	D	1100	4.155	9.281	-45.042	1.00 45.57	RNA2 O
ATOM	3822	C3*	C	D	1100	4.502	9.335	-47.356	1.00 48.34	RNA2 C
ATOM	3823	O3*	C	D	1100	4.774	10.136	-48.495	1.00 58.69	RNA2 O
ATOM	3824	C2*	C	D	1100	5.771	8.784	-46.718	1.00 42.72	RNA2 C
ATOM	3825	O2*	C	D	1100	6.840	9.707	-46.670	1.00 45.27	RNA2 O
ATOM	3826	C1*	C	D	1100	5.289	8.466	-45.303	1.00 36.28	RNA2 C
ATOM	3827	N1	C	D	1100	4.897	7.048	-45.234	1.00 33.17	RNA2 N
ATOM	3828	C2	C	D	1100	5.910	6.083	-45.177	1.00 37.72	RNA2 C
ATOM	3829	O2	C	D	1100	7.090	6.461	-45.104	1.00 37.78	RNA2 O
ATOM	3830	N3	C	D	1100	5.582	4.772	-45.201	1.00 34.10	RNA2 N
ATOM	3831	C4	C	D	1100	4.299	4.409	-45.268	1.00 36.21	RNA2 C
ATOM	3832	N4	C	D	1100	4.024	3.103	-45.330	1.00 35.52	RNA2 N
ATOM	3833	C5	C	D	1100	3.242	5.369	-45.283	1.00 32.04	RNA2 C
ATOM	3834	C6	C	D	1100	3.583	6.665	-45.263	1.00 33.05	RNA2 C
ATOM	3835	P	U	D	1101	4.754	9.460	-49.951	1.00 59.64	RNA2 P
ATOM	3836	O1P	U	D	1101	3.464	8.731	-50.077	1.00 53.79	RNA2 O
ATOM	3837	O2P	U	D	1101	5.117	10.490	-50.957	1.00 73.54	RNA2 O
ATOM	3838	O5*	U	D	1101	5.931	8.390	-49.894	1.00 44.03	RNA2 O
ATOM	3839	C5*	U	D	1101	7.275	8.809	-49.652	1.00 37.19	RNA2 C
ATOM	3840	C4*	U	D	1101	8.197	7.620	-49.625	1.00 44.44	RNA2 C
ATOM	3841	O4*	U	D	1101	7.844	6.748	-48.520	1.00 47.50	RNA2 O
ATOM	3842	C3*	U	D	1101	8.140	6.710	-50.836	1.00 49.53	RNA2 C
ATOM	3843	O3*	U	D	1101	8.892	7.203	-51.930	1.00 55.95	RNA2 O
ATOM	3844	C2*	U	D	1101	8.681	5.396	-50.286	1.00 46.03	RNA2 C
ATOM	3845	O2*	U	D	1101	10.091	5.371	-50.196	1.00 46.23	RNA2 O
ATOM	3846	C1*	U	D	1101	8.097	5.396	-48.875	1.00 41.37	RNA2 C
ATOM	3847	N1	U	D	1101	6.840	4.627	-48.800	1.00 33.41	RNA2 N
ATOM	3848	C2	U	D	1101	6.935	3.238	-48.784	1.00 34.44	RNA2 C
ATOM	3849	O2	U	D	1101	8.011	2.640	-48.812	1.00 33.60	RNA2 O
ATOM	3850	N3	U	D	1101	5.730	2.575	-48.737	1.00 17.93	RNA2 N
ATOM	3851	C4	U	D	1101	4.466	3.143	-48.705	1.00 36.01	RNA2 C
ATOM	3852	O4	U	D	1101	3.465	2.411	-48.702	1.00 25.00	RNA2 O
ATOM	3853	C5	U	D	1101	4.457	4.577	-48.714	1.00 24.85	RNA2 C
ATOM	3854	C6	U	D	1101	5.610	5.251	-48.760	1.00 26.88	RNA2 C
ATOM	3855	P	C	D	1102	8.485	6.763	-53.418	1.00 41.89	RNA2 P
ATOM	3856	O1P	C	D	1102	7.001	6.821	-53.510	1.00 43.20	RNA2 O
ATOM	3857	O2P	C	D	1102	9.312	7.542	-54.372	1.00 53.94	RNA2 O
ATOM	3858	O5*	C	D	1102	8.938	5.240	-53.483	1.00 38.14	RNA2 O
ATOM	3859	C5*	C	D	1102	10.317	4.889	-53.306	1.00 37.05	RNA2 C
ATOM	3860	C4*	C	D	1102	10.494	3.390	-53.332	1.00 45.27	RNA2 C
ATOM	3861	O4*	C	D	1102	9.855	2.793	-52.168	1.00 52.28	RNA2 O
ATOM	3862	C3*	C	D	1102	9.872	2.637	-54.498	1.00 54.50	RNA2 C

ATOM	3863	O3*	C	D1102	10.597	2.706	-55.716	1.00	57.12	RNA2	O
ATOM	3864	C2*	C	D1102	9.784	1.219	-53.949	1.00	52.66	RNA2	C
ATOM	3865	O2*	C	D1102	11.017	0.522	-54.000	1.00	56.57	RNA2	O
ATOM	3866	C1*	C	D1102	9.401	1.482	-52.493	1.00	46.15	RNA2	C
ATOM	3867	N1	C	D1102	7.932	1.399	-52.330	1.00	28.20	RNA2	N
ATOM	3868	C2	C	D1102	7.331	0.128	-52.307	1.00	22.69	RNA2	C
ATOM	3869	O2	C	D1102	8.053	-0.881	-52.366	1.00	35.31	RNA2	O
ATOM	3870	N3	C	D1102	5.988	0.028	-52.219	1.00	9.49	RNA2	N
ATOM	3871	C4	C	D1102	5.246	1.129	-52.135	1.00	16.43	RNA2	C
ATOM	3872	N4	C	D1102	3.922	0.979	-52.052	1.00	15.53	RNA2	N
ATOM	3873	C5	C	D1102	5.825	2.433	-52.133	1.00	15.77	RNA2	C
ATOM	3874	C6	C	D1102	7.158	2.521	-52.229	1.00	21.76	RNA2	C
ATOM	3875	P	A	D1103	9.806	2.525	-57.105	1.00	47.42	RNA2	P
ATOM	3876	O1P	A	D1103	8.514	3.264	-57.011	1.00	38.37	RNA2	O
ATOM	3877	O2P	A	D1103	10.747	2.818	-58.216	1.00	57.18	RNA2	O
ATOM	3878	O5*	A	D1103	9.456	0.974	-57.138	1.00	48.19	RNA2	O
ATOM	3879	C5*	A	D1103	10.493	-0.015	-56.995	1.00	51.39	RNA2	C
ATOM	3880	C4*	A	D1103	9.894	-1.397	-56.965	1.00	45.50	RNA2	C
ATOM	3881	O4*	A	D1103	8.978	-1.488	-55.847	1.00	45.01	RNA2	O
ATOM	3882	C3*	A	D1103	9.053	-1.764	-58.178	1.00	51.96	RNA2	C
ATOM	3883	O3*	A	D1103	9.867	-2.246	-59.243	1.00	53.83	RNA2	O
ATOM	3884	C2*	A	D1103	8.095	-2.817	-57.622	1.00	48.46	RNA2	C
ATOM	3885	O2*	A	D1103	8.635	-4.125	-57.578	1.00	47.52	RNA2	O
ATOM	3886	C1*	A	D1103	7.882	-2.316	-56.192	1.00	43.28	RNA2	C
ATOM	3887	N9	A	D1103	6.646	-1.549	-56.032	1.00	30.89	RNA2	N
ATOM	3888	C8	A	D1103	6.477	-0.189	-55.914	1.00	25.35	RNA2	C
ATOM	3889	N7	A	D1103	5.222	0.179	-55.797	1.00	26.03	RNA2	N
ATOM	3890	C5	A	D1103	4.519	-1.019	-55.836	1.00	17.17	RNA2	C
ATOM	3891	C6	A	D1103	3.149	-1.314	-55.759	1.00	19.87	RNA2	C
ATOM	3892	N6	A	D1103	2.193	-0.387	-55.623	1.00	16.79	RNA2	N
ATOM	3893	N1	A	D1103	2.784	-2.616	-55.828	1.00	26.16	RNA2	N
ATOM	3894	C2	A	D1103	3.737	-3.548	-55.965	1.00	23.04	RNA2	C
ATOM	3895	N3	A	D1103	5.055	-3.394	-56.049	1.00	30.58	RNA2	N
ATOM	3896	C4	A	D1103	5.384	-2.090	-55.977	1.00	28.62	RNA2	C
ATOM	3897	P	C	D1104	9.699	-1.627	-60.718	1.00	44.57	RNA2	P
ATOM	3898	O1P	C	D1104	9.942	-0.162	-60.644	1.00	47.15	RNA2	O
ATOM	3899	O2P	C	D1104	10.506	-2.463	-61.648	1.00	47.11	RNA2	O
ATOM	3900	O5*	C	D1104	8.160	-1.850	-61.042	1.00	36.26	RNA2	O
ATOM	3901	C5*	C	D1104	7.642	-3.172	-61.211	1.00	34.08	RNA2	C
ATOM	3902	C4*	C	D1104	6.144	-3.130	-61.321	1.00	33.02	RNA2	C
ATOM	3903	O4*	C	D1104	5.569	-2.739	-60.048	1.00	35.45	RNA2	O
ATOM	3904	C3*	C	D1104	5.595	-2.113	-62.301	1.00	36.26	RNA2	C
ATOM	3905	O3*	C	D1104	5.633	-2.561	-63.643	1.00	42.96	RNA2	O
ATOM	3906	C2*	C	D1104	4.183	-1.890	-61.780	1.00	35.20	RNA2	C
ATOM	3907	O2*	C	D1104	3.297	-2.916	-62.185	1.00	38.85	RNA2	O

ATOM	3908	C1*	C	D1104	4.408	-1.952	-60.268	1.00	31.46	RNA2	C
ATOM	3909	N1	C	D1104	4.636	-0.606	-59.702	1.00	26.13	RNA2	N
ATOM	3910	C2	C	D1104	3.528	0.178	-59.334	1.00	24.36	RNA2	C
ATOM	3911	O2	C	D1104	2.386	-0.295	-59.447	1.00	21.42	RNA2	O
ATOM	3912	N3	C	D1104	3.735	1.428	-58.865	1.00	27.00	RNA2	N
ATOM	3913	C4	C	D1104	4.981	1.900	-58.745	1.00	31.66	RNA2	C
ATOM	3914	N4	C	D1104	5.140	3.147	-58.292	1.00	37.50	RNA2	N
ATOM	3915	C5	C	D1104	6.120	1.119	-59.087	1.00	19.85	RNA2	C
ATOM	3916	C6	C	D1104	5.906	-0.115	-59.554	1.00	26.62	RNA2	C
ATOM	3917	P	C	D1105	5.825	-1.489	-64.826	1.00	42.78	RNA2	P
ATOM	3918	O1P	C	D1105	6.805	-0.460	-64.381	1.00	36.29	RNA2	O
ATOM	3919	O2P	C	D1105	6.074	-2.246	-66.084	1.00	51.04	RNA2	O
ATOM	3920	O5*	C	D1105	4.397	-0.802	-64.932	1.00	18.59	RNA2	O
ATOM	3921	C5*	C	D1105	3.253	-1.574	-65.316	1.00	29.02	RNA2	C
ATOM	3922	C4*	C	D1105	2.021	-0.711	-65.320	1.00	36.00	RNA2	C
ATOM	3923	O4*	C	D1105	1.741	-0.275	-63.965	1.00	45.01	RNA2	O
ATOM	3924	C3*	C	D1105	2.122	0.582	-66.111	1.00	43.97	RNA2	C
ATOM	3925	O3*	C	D1105	1.919	0.405	-67.505	1.00	50.57	RNA2	O
ATOM	3926	C2*	C	D1105	1.060	1.451	-65.447	1.00	42.61	RNA2	C
ATOM	3927	O2*	C	D1105	-0.259	1.147	-65.873	1.00	33.02	RNA2	O
ATOM	3928	C1*	C	D1105	1.225	1.048	-63.983	1.00	40.14	RNA2	C
ATOM	3929	N1	C	D1105	2.173	1.938	-63.273	1.00	34.85	RNA2	N
ATOM	3930	C2	C	D1105	1.704	3.161	-62.765	1.00	30.45	RNA2	C
ATOM	3931	O2	C	D1105	0.516	3.473	-62.939	1.00	29.26	RNA2	O
ATOM	3932	N3	C	D1105	2.558	3.975	-62.106	1.00	32.19	RNA2	N
ATOM	3933	C4	C	D1105	3.836	3.622	-61.956	1.00	39.46	RNA2	C
ATOM	3934	N4	C	D1105	4.644	4.466	-61.298	1.00	41.48	RNA2	N
ATOM	3935	C5	C	D1105	4.346	2.391	-62.471	1.00	36.86	RNA2	C
ATOM	3936	C6	C	D1105	3.488	1.587	-63.114	1.00	34.30	RNA2	C
ATOM	3937	P	A	D1106	2.559	1.463	-68.538	1.00	47.42	RNA2	P
ATOM	3938	O1P	A	D1106	3.960	1.743	-68.117	1.00	33.03	RNA2	O
ATOM	3939	O2P	A	D1106	2.297	0.944	-69.905	1.00	51.03	RNA2	O
ATOM	3940	O5*	A	D1106	1.674	2.772	-68.323	1.00	38.12	RNA2	O
ATOM	3941	C5*	A	D1106	0.283	2.777	-68.706	1.00	43.96	RNA2	C
ATOM	3942	C4*	A	D1106	-0.340	4.129	-68.452	1.00	51.41	RNA2	C
ATOM	3943	O4*	A	D1106	-0.379	4.381	-67.026	1.00	57.25	RNA2	O
ATOM	3944	C3*	A	D1106	0.391	5.331	-69.029	1.00	56.31	RNA2	C
ATOM	3945	O3*	A	D1106	0.086	5.559	-70.396	1.00	55.12	RNA2	O
ATOM	3946	C2*	A	D1106	-0.076	6.467	-68.126	1.00	56.95	RNA2	C
ATOM	3947	O2*	A	D1106	-1.351	6.970	-68.478	1.00	57.32	RNA2	O
ATOM	3948	C1*	A	D1106	-0.169	5.761	-66.776	1.00	49.81	RNA2	C
ATOM	3949	N9	A	D1106	1.065	5.896	-66.003	1.00	39.90	RNA2	N
ATOM	3950	C8	A	D1106	2.098	4.994	-65.902	1.00	41.00	RNA2	C
ATOM	3951	N7	A	D1106	3.070	5.388	-65.116	1.00	41.71	RNA2	N
ATOM	3952	C5	A	D1106	2.652	6.635	-64.672	1.00	37.31	RNA2	C

ATOM	3953	C6	A	D1106	3.238	7.572	-63.805	1.00	36.44	RNA2 C
ATOM	3954	N6	A	D1106	4.419	7.389	-63.208	1.00	40.12	RNA2 N
ATOM	3955	N1	A	D1106	2.563	8.720	-63.570	1.00	38.29	RNA2 N
ATOM	3956	C2	A	D1106	1.380	8.904	-64.178	1.00	37.00	RNA2 C
ATOM	3957	N3	A	D1106	0.726	8.097	-65.014	1.00	37.07	RNA2 N
ATOM	3958	C4	A	D1106	1.423	6.965	-65.219	1.00	37.01	RNA2 C
ATOM	3959	P	G	D1107	1.186	6.251	-71.341	1.00	60.89	RNA2 P
ATOM	3960	O1P	G	D1107	2.513	5.650	-71.037	1.00	51.64	RNA2 O
ATOM	3961	O2P	G	D1107	0.665	6.218	-72.732	1.00	66.72	RNA2 O
ATOM	3962	O5*	G	D1107	1.226	7.763	-70.838	1.00	59.43	RNA2 O
ATOM	3963	C5*	G	D1107	0.098	8.639	-71.043	1.00	70.93	RNA2 C
ATOM	3964	C4*	G	D1107	0.341	9.984	-70.392	1.00	70.62	RNA2 C
ATOM	3965	O4*	G	D1107	0.347	9.841	-68.945	1.00	70.80	RNA2 O
ATOM	3966	C3*	G	D1107	1.673	10.648	-70.701	1.00	69.85	RNA2 C
ATOM	3967	O3*	G	D1107	1.703	11.337	-71.937	1.00	68.76	RNA2 O
ATOM	3968	C2*	G	D1107	1.852	11.589	-69.519	1.00	71.85	RNA2 C
ATOM	3969	O2*	G	D1107	1.134	12.799	-69.666	1.00	74.63	RNA2 O
ATOM	3970	C1*	G	D1107	1.278	10.751	-68.377	1.00	66.31	RNA2 C
ATOM	3971	N9	G	D1107	2.356	9.990	-67.753	1.00	61.03	RNA2 N
ATOM	3972	C8	G	D1107	2.765	8.710	-68.056	1.00	64.56	RNA2 C
ATOM	3973	N7	G	D1107	3.811	8.330	-67.371	1.00	62.08	RNA2 N
ATOM	3974	C5	G	D1107	4.100	9.417	-66.555	1.00	59.12	RNA2 C
ATOM	3975	C6	G	D1107	5.134	9.600	-65.598	1.00	54.80	RNA2 C
ATOM	3976	O6	G	D1107	6.035	8.812	-65.270	1.00	51.34	RNA2 O
ATOM	3977	N1	G	D1107	5.056	10.854	-65.001	1.00	50.79	RNA2 N
ATOM	3978	C2	G	D1107	4.109	11.810	-65.287	1.00	54.33	RNA2 C
ATOM	3979	N2	G	D1107	4.199	12.959	-64.606	1.00	51.64	RNA2 N
ATOM	3980	N3	G	D1107	3.146	11.653	-66.176	1.00	49.03	RNA2 N
ATOM	3981	C4	G	D1107	3.201	10.443	-66.769	1.00	58.09	RNA2 C
ATOM	3982	P	C	D1108	3.118	11.599	-72.654	1.00	71.56	RNA2 P
ATOM	3983	O1P	C	D1108	3.923	10.353	-72.579	1.00	60.79	RNA2 O
ATOM	3984	O2P	C	D1108	2.828	12.209	-73.977	1.00	78.78	RNA2 O
ATOM	3985	O5*	C	D1108	3.837	12.677	-71.723	1.00	69.28	RNA2 O
ATOM	3986	C5*	C	D1108	3.274	13.992	-71.536	1.00	65.61	RNA2 C
ATOM	3987	C4*	C	D1108	4.139	14.809	-70.605	1.00	60.04	RNA2 C
ATOM	3988	O4*	C	D1108	4.193	14.171	-69.304	1.00	61.74	RNA2 O
ATOM	3989	C3*	C	D1108	5.598	14.965	-71.001	1.00	60.53	RNA2 C
ATOM	3990	O3*	C	D1108	5.901	15.783	-72.134	1.00	66.71	RNA2 O
ATOM	3991	C2*	C	D1108	6.282	15.272	-69.677	1.00	63.96	RNA2 C
ATOM	3992	O2*	C	D1108	6.155	16.631	-69.306	1.00	69.72	RNA2 O
ATOM	3993	C1*	C	D1108	5.457	14.420	-68.706	1.00	64.54	RNA2 C
ATOM	3994	N1	C	D1108	6.098	13.130	-68.372	1.00	61.20	RNA2 N
ATOM	3995	C2	C	D1108	7.127	13.116	-67.417	1.00	59.89	RNA2 C
ATOM	3996	O2	C	D1108	7.454	14.179	-66.867	1.00	54.39	RNA2 O
ATOM	3997	N3	C	D1108	7.739	11.946	-67.119	1.00	60.31	RNA2 N

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ATOM   3998  C4    C D1108      7.359  10.821 -67.728  1.00 62.68      RNA2 C
ATOM   3999  N4    C D1108      7.999   9.689 -67.411  1.00 63.03      RNA2 N
ATOM   4000  C5    C D1108      6.308  10.803 -68.693  1.00 64.65      RNA2 C
ATOM   4001  C6    C D1108      5.711  11.968 -68.982  1.00 64.25      RNA2 C
TER    4002        C D1108
HETATM 4003 CD   CD  201       4.250  -2.291  -5.735  0.91 77.47       CD
HETATM 4004 CD   CD  202       5.716   1.827   1.431  0.91 32.35       CD
HETATM 4005  O   HOH  205       7.540  -4.792  -0.436  1.00 19.29       O
HETATM 4006  O   HOH  209       8.097   9.026  -9.315  1.00 27.99       O
HETATM 4007 MG   MG  210       7.174   1.073 -14.750  1.00 31.99       MG
HETATM 4008 CD   CD  211       3.380   6.488 -27.905  0.91 47.98       CD
HETATM 4009  O   HOH  213      -0.304   4.175  -0.867  1.00 38.63       O
HETATM 4010 MG   MG  214     -17.505  21.323  11.148  1.00 36.28       MG
HETATM 4011 MG   MG  215      -1.702   7.910 -11.196  1.00 23.07       MG
HETATM 4012  O   HOH  216      -3.510   9.209 -16.056  1.00 43.93       O
HETATM 4013  O   HOH  217      -4.416  -0.858  -2.563  1.00 53.29       O
HETATM 4014  O   HOH  218       6.288  -5.327  -3.385  1.00 23.44       O
HETATM 4015  O   HOH  221      -1.778   1.682  -3.132  1.00 35.80       O
HETATM 4016  O   HOH  222      -6.849  10.117  -5.442  1.00 24.81       O
HETATM 4017 MG   MG  223      14.749  -5.902  12.250  1.00 36.97       MG
HETATM 4018 MG   MG  225      19.765  -8.266  10.030  1.00 41.29       MG
HETATM 4019 MG   MG  226       4.983   5.583 -14.224  1.00 17.24       MG
HETATM 4020 HG   HG  227      10.163  10.934  -4.731  0.10 21.14       HG
HETATM 4021 MG   MG  228       0.368  -4.197  15.065  1.00 49.67       MG
HETATM 4022 HG   HG  230      -4.955   2.266 -15.287  0.41 65.01       HG
HETATM 4023  O   HOH  232      17.184  -8.123  12.078  1.00 46.90       O
HETATM 4024  O   HOH  233       5.132  -9.156  11.493  1.00 39.77       O
HETATM 4025  O   HOH  235      -2.182   2.520  -0.424  1.00 32.75       O
HETATM 4026  O   HOH  236       3.337   3.950  -2.832  1.00 22.74       O
HETATM 4027  O   HOH  237      -0.294   3.992  -4.949  1.00 41.19       O
HETATM 4028  O   HOH  238       3.987   7.706  -7.271  1.00 22.33       O
HETATM 4029  O   HOH  239      -2.682   1.061 -25.220  1.00 28.52       O
HETATM 4030  O   HOH  241      -0.901  -1.716  11.637  1.00 34.24       O
HETATM 4031  O   HOH  243      13.905 -12.456   1.182  1.00 61.18       O
HETATM 4032  O   HOH  244      -6.595   6.151   4.226  1.00 33.67       O
HETATM 4033  O   HOH  245     -10.614  11.084  18.691  1.00 47.29       O
HETATM 4034  O   HOH  246       2.153   6.645  -5.263  1.00 42.17       O
HETATM 4035  O   HOH  254       1.596   7.517 -28.596  1.00 20.43       O
HETATM 4036  O   HOH  255       5.496   5.982 -27.129  1.00 15.56       O
HETATM 4037  O   HOH  256       5.082   7.342 -29.082  1.00 15.30       O
HETATM 4038 MG   MG  257       4.272   8.284 -11.053  1.00 18.63       MG
HETATM 4039  O   HOH  258       5.759   9.095  -9.332  1.00 22.95       O
HETATM 4040  O   HOH  259       5.439   8.750 -13.001  1.00 29.22       O
HETATM 4041  O   HOH  260       3.112   6.893  -9.834  1.00 15.63       O
HETATM 4042  O   HOH  261       2.565   9.752 -11.319  1.00 21.45       O
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HETATM 4043  O   HOH  262      2.003  -1.889  -6.293  1.00 39.08           O
HETATM 4044  O   HOH  263      6.523  -2.887  -3.470  1.00 31.47           O
HETATM 4045  O   HOH  264      5.691  -4.152  -6.413  1.00 49.36           O
HETATM 4046  O   HOH  265     13.164  -1.037 -13.541  1.00 53.81           O
HETATM 4047  O   HOH  266      1.658  -4.440  -6.534  1.00 54.55           O
HETATM 4048  O   HOH  267      4.147  -0.985 -10.097  1.00 21.21           O
HETATM 4049  O   HOH  268      7.729   0.998 -17.041  1.00 32.76           O
HETATM 4050  O   HOH  269      9.473   0.412 -15.439  1.00 22.86           O
HETATM 4051  O   HOH  270      5.281   1.436 -15.928  1.00 30.01           O
HETATM 4052  O   HOH  271      5.086  -1.392 -12.878  1.00 29.98           O
HETATM 4053  O   HOH  272      5.284  18.973 -15.526  1.00 29.56           O
HETATM 4054 MG   MG   273      5.268   8.632   9.371  1.00 35.80          MG
HETATM 4055  O   HOH  274      4.009   8.265   7.258  1.00 21.81           O
HETATM 4056  O   HOH  275      6.536   8.905   7.475  1.00 34.86           O
HETATM 4057  O   HOH  276      3.058   8.060   9.657  1.00 31.13           O
HETATM 4058  O   HOH  277      5.081   6.362   8.463  1.00 31.02           O
HETATM 4059  O   HOH  278      3.600  10.499   8.517  1.00 50.03           O
HETATM 4060 CD   CD   302      0.011  -4.071 -53.380  0.91 31.52          CD
HETATM 4061  O   HOH  305      1.845   2.702 -51.597  1.00 14.19           O
HETATM 4062 CD   CD   311      4.100  -9.327 -24.111  0.91 76.29          CD
HETATM 4063  O   HOH  313     -1.010  -7.500 -47.833  1.00 40.72           O
HETATM 4064 MG   MG   318      1.219   3.097 -48.942  1.00 17.48          MG
HETATM 4065  O   HOH  322    -10.157 -13.890 -44.431  1.00 41.81           O
HETATM 4066 MG   MG   326      2.778  -7.878 -38.005  1.00 11.66          MG
HETATM 4067  O   HOH  327      9.652  -2.170 -38.994  1.00 44.35           O
HETATM 4068 HG   HG   332     -7.089  -5.545 -35.006  0.60 82.38          HG
HETATM 4069  O   HOH  333      1.493 -12.458 -57.479  1.00 39.19           O
HETATM 4070  O   HOH  335     -4.211   7.242 -62.792  1.00 49.93           O
HETATM 4071  O   HOH  336     -7.759  -5.212 -49.585  1.00 35.75           O
HETATM 4072  O   HOH  338     -3.953  -6.679 -45.543  1.00 38.41           O
HETATM 4073  O   HOH  339      0.508 -10.010 -44.801  1.00 28.38           O
HETATM 4074  O   HOH  340     -8.610   1.401 -65.472  1.00 31.42           O
HETATM 4075  O   HOH  343      5.058 -10.891 -43.391  1.00 29.07           O
HETATM 4076  O   HOH  345      5.817 -19.070 -33.612  1.00 35.77           O
HETATM 4077  O   HOH  346      8.758 -14.281 -46.244  1.00 40.41           O
HETATM 4078 HG   HG   347      6.715 -12.669 -48.448  0.20 54.24          HG
HETATM 4079  O   HOH  349      5.113 -13.530 -54.095  1.00 42.05           O
HETATM 4080  O   HOH  352      6.195  -6.263 -57.438  1.00 39.69           O
HETATM 4081  O   HOH  353     12.125   3.149 -49.649  1.00 38.23           O
HETATM 4082 MG   MG   354     11.145   8.122 -61.981  1.00 29.67          MG
HETATM 4083  O   HOH  355     10.792   7.517 -64.576  1.00 68.09           O
HETATM 4084  O   HOH  356     12.630   7.721 -60.264  1.00 42.56           O
HETATM 4085  O   HOH  357     13.374   7.731 -62.491  1.00 44.36           O
HETATM 4086  O   HOH  358      8.902   7.560 -61.857  1.00 47.98           O
HETATM 4087 MG   MG   360      6.237   6.431 -66.914  1.00 28.74          MG
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HETATM	4088	O	HOH	361	6.408	4.325	-65.550	1.00	56.01	O
HETATM	4089	O	HOH	362	8.361	5.765	-66.746	1.00	36.18	O
HETATM	4090	O	HOH	363	4.653	5.030	-68.186	1.00	40.11	O
HETATM	4091	O	HOH	364	7.146	6.368	-64.453	1.00	50.71	O
HETATM	4092	MG	MG	365	4.856	8.795	-57.034	1.00	57.29	MG
HETATM	4093	O	HOH	367	5.981	7.693	-58.709	1.00	45.32	O
HETATM	4094	O	HOH	368	2.602	9.503	-57.044	1.00	34.21	O
HETATM	4095	O	HOH	369	-3.740	-7.741	-49.878	1.00	34.52	O
HETATM	4096	O	HOH	371	-4.630	-7.088	-47.848	1.00	47.42	O
HETATM	4097	O	HOH	372	-1.660	-6.106	-49.542	1.00	29.15	O
HETATM	4098	O	HOH	373	-6.163	-7.124	-50.377	1.00	43.85	O
HETATM	4099	O	HOH	374	-4.330	-5.161	-49.766	1.00	36.71	O
HETATM	4100	MG	MG	375	-4.006	-10.777	-39.969	1.00	19.68	MG
HETATM	4101	O	HOH	376	-3.858	-12.278	-36.949	1.00	28.95	O
HETATM	4102	O	HOH	377	-2.097	-12.249	-40.683	1.00	38.24	O
HETATM	4103	O	HOH	378	-5.782	-11.177	-38.567	1.00	48.85	O
HETATM	4104	O	HOH	379	-3.396	-9.585	-37.760	1.00	53.51	O
HETATM	4105	MG	MG	380	1.544	-10.560	-40.973	1.00	15.03	MG
HETATM	4106	O	HOH	381	0.239	-9.278	-41.992	1.00	24.23	O
HETATM	4107	O	HOH	382	3.079	-11.151	-39.552	1.00	29.52	O
HETATM	4108	O	HOH	383	2.890	-11.254	-42.623	1.00	28.59	O
HETATM	4109	O	HOH	384	0.497	-12.218	-40.320	1.00	24.46	O
HETATM	4110	MG	MG	385	4.975	-3.399	-36.540	1.00	26.05	MG
HETATM	4111	O	HOH	386	4.351	-3.722	-38.893	1.00	47.91	O
HETATM	4112	O	HOH	387	6.538	-3.279	-34.525	1.00	52.58	O
HETATM	4113	O	HOH	388	6.829	-2.324	-37.582	1.00	23.58	O
HETATM	4114	O	HOH	389	2.776	-4.208	-36.379	1.00	47.45	O
HETATM	4115	CD	CD	390	-0.220	-0.169	-45.971	1.00	66.34	CD
HETATM	4116	O	HOH	391	1.204	0.456	-48.678	1.00	26.12	O
HETATM	4117	O	HOH	392	-2.039	-0.298	-44.457	1.00	74.79	O
HETATM	4118	O	HOH	394	-2.332	-1.375	-46.858	1.00	55.72	O
HETATM	4119	O	HOH	395	0.735	-1.415	-41.666	1.00	23.21	O
HETATM	4120	O	HOH	396	-2.289	1.508	-46.080	1.00	38.73	O
HETATM	4121	MG	MG	397	-1.117	-10.966	-60.412	1.00	36.18	MG
HETATM	4122	O	HOH	399	-2.144	-9.538	-58.861	1.00	29.70	O
HETATM	4123	O	HOH	400	1.112	-10.642	-59.923	1.00	66.19	O
HETATM	4124	O	HOH	401	-3.291	-10.503	-60.904	1.00	35.31	O
HETATM	4125	O	HOH	402	-2.294	-12.413	-59.078	1.00	39.66	O
HETATM	4126	O	HOH	403	-1.467	-8.797	-61.459	1.00	53.05	O
HETATM	4127	O	HOH	404	-12.040	-30.139	-41.430	1.00	41.13	O
HETATM	4128	O	HOH	405	-2.445	-24.982	-35.646	1.00	41.49	O
HETATM	4129	O	HOH	406	-12.232	-9.609	-53.785	1.00	19.82	O
HETATM	4130	O	HOH	407	-10.736	-14.577	-49.559	1.00	27.37	O
HETATM	4131	O	HOH	408	-18.946	-19.067	-62.962	1.00	48.41	O
HETATM	4132	O	HOH	409	-19.414	-10.463	-60.502	1.00	52.79	O

HETATM	4133	O	HOH	410	-6.651	-19.456	-54.939	1.00	26.78	O
HETATM	4134	O	HOH	411	-2.899	-18.491	-49.891	1.00	31.34	O
HETATM	4135	O	HOH	412	-4.041	-25.738	-47.368	1.00	61.51	O
HETATM	4136	CD	CD	413	-13.027	8.492	10.933	0.10	33.43	CD
HETATM	4137	CD	CD	414	-11.592	5.003	-2.412	0.10	14.13	CD
HETATM	4138	HG	HG	415	-23.456	-2.491	-20.626	0.10	35.19	HG
HETATM	4139	HG	HG	416	-17.183	-2.624	-19.816	0.10	45.02	HG
HETATM	4140	O	HOH	418	-0.113	29.557	-9.189	1.00	36.18	O
HETATM	4141	O	HOH	419	-1.958	16.568	4.135	1.00	22.82	O
HETATM	4142	O	HOH	420	0.874	15.995	-1.216	1.00	36.22	O
HETATM	4143	O	HOH	421	-0.098	21.800	-5.101	1.00	35.12	O
HETATM	4144	O	HOH	422	-1.412	23.130	-2.906	1.00	36.67	O
HETATM	4145	O	HOH	423	-3.317	24.792	0.592	1.00	45.31	O
HETATM	4146	O	HOH	424	0.019	9.295	-10.598	1.00	36.37	O
HETATM	4147	O	HOH	425	-2.568	8.364	-13.958	1.00	50.92	O
HETATM	4148	O	HOH	426	-2.689	18.373	-24.066	1.00	34.21	O
HETATM	4149	O	HOH	427	7.170	6.156	-29.910	1.00	17.29	O
HETATM	4150	O	HOH	428	8.929	4.171	-22.749	1.00	41.67	O
HETATM	4151	O	HOH	429	12.036	0.863	-14.965	1.00	42.52	O
HETATM	4152	O	HOH	431	-1.202	8.279	12.504	1.00	41.33	O
HETATM	4153	O	HOH	432	8.485	7.265	7.104	1.00	46.57	O
HETATM	4154	O	HOH	434	4.018	10.172	4.758	1.00	37.32	O
HETATM	4155	O	HOH	435	18.225	-9.006	-2.120	1.00	60.80	O
HETATM	4156	MG	MG	437	11.760	-10.915	4.311	1.00	47.79	MG
HETATM	4157	O	HOH	438	12.113	-10.561	1.951	1.00	58.11	O
HETATM	4158	O	HOH	440	14.043	-10.435	3.845	1.00	43.62	O
HETATM	4159	O	HOH	441	9.524	-10.398	4.381	1.00	41.20	O
HETATM	4160	O	HOH	442	11.946	-13.321	4.538	1.00	65.98	O
HETATM	4161	O	HOH	443	12.227	-8.461	4.164	1.00	61.70	O
HETATM	4162	O	HOH	444	1.040	4.817	-2.689	1.00	32.93	O
HETATM	4163	O	HOH	445	4.226	0.914	2.202	1.00	3.57	O
HETATM	4164	O	HOH	446	6.340	-0.071	1.151	1.00	19.50	O
HETATM	4165	O	HOH	447	4.234	3.232	1.596	1.00	12.18	O
HETATM	4166	HG	HG	448	-4.015	-8.066	-15.150	0.10	21.04	HG
HETATM	4167	O	HOH	450	-4.907	-3.163	-52.117	1.00	24.48	O
HETATM	4168	HG	HG	451	-5.485	5.932	-35.358	0.10	26.20	HG
HETATM	4169	O	HOH	452	-4.427	1.650	-44.668	1.00	47.88	O
HETATM	4170	O	HOH	453	-6.126	-4.197	-47.630	1.00	40.28	O
HETATM	4171	O	HOH	454	-14.902	-5.184	-53.399	1.00	41.04	O
HETATM	4172	O	HOH	455	2.198	-31.615	-45.895	1.00	38.45	O
HETATM	4173	O	HOH	456	-0.111	-29.053	-48.914	1.00	37.64	O
HETATM	4174	O	HOH	457	5.023	-28.677	-39.390	1.00	42.30	O
HETATM	4175	O	HOH	459	-8.700	-0.565	-36.045	1.00	32.85	O
HETATM	4176	O	HOH	460	-1.593	-4.423	-51.572	1.00	28.40	O
HETATM	4177	O	HOH	461	-1.729	-3.181	-53.813	1.00	2.00	O

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HETATM 4178  O   HOH  462     -1.294  -5.593 -53.672  1.00 22.25           O
HETATM 4179  O   HOH  463      0.388  -1.958 -53.133  1.00 27.43           O
MASTER      320    0   35    8    7    0    3   12 4175    4    0   32
END
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